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EVALUATION OF A PHYSIOLOGICALLY-BASED PHARMACOKINETIC (PBPK) MODEL USED TO DEVELOP HEALTH PROTECTIVE LEVELS FOR TRICHLOROETHYLENE

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Evaluation of a Physiologically-Based Pharmacokinetic (PBPK) Model Used To Develop Health Protective Levels For Trichloroethylene

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14. ABSTRACT
Trichloroethylene (TCE) was commonly used as a solvent by the Department of Defense (DoD), as well at private sector facilities. Releases to the environment from its past use make TCE one of the most common contaminants encountered at hazardous waste sites. The Air Force Research Laboratory previously worked with the U.S. Environmental Protection Agency (EPA) to develop a harmonized physiologically-based pharmacokinetic (PBPK) model for TCE; the model was updated by EPA for their use in their toxicological review. An evaluation of the updated PBPK model will provide insight into the uncertainty associated with its use by EPA. The evaluation involved the following tasks: 1) obtain the PBPK model EPA used in its Toxicological Review of Trichloroethylene dated September 2011 and demonstrate that the model may be validated; 2) perform a sensitivity analysis and in that assessment include an evaluation of EPA's Bayesian method for prior validation and impact of their use of the method (see Appendix A of the Toxicological Review); and 3) develop deliverables describing the methods used and the outcomes of each of these tasks. The methods used to complete these tasks and the resulting findings are presented in this report. Model instability and error are discussed and recommendations are noted.

15. SUBJECT TERMS
trichloroethylene, contamination, physiologically-based pharmacokinetic model, evaluation, PBPK, solvent, TCE, sensitivity analysis

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PREFACE

Funding for this effort was provided by the U.S. Army Engineering & Support Center, the Air Force Civil Engineering Center (AFCEC), and the Aerospace Toxicology Program, which is part of the Aerospace Physiology and Toxicology Program in the 711th Human Performance Wing of the Air Force Research Laboratory. This research was conducted under a cooperative agreement FA8650-15-2-6608 with the Henry M. Jackson Foundation for the Advancement of Military Medicine (HJF). The program manager for the HJF cooperative agreement was David R. Mattie, PhD (711 HPW/RHDJ), who was also the technical manager for this project.

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1.0 SUMMARY

Trichloroethylene (TCE) was commonly used as a solvent by the Department of Defense (DoD), as well as at private sector facilities. Releases to the environment from its past use make TCE one of the most common contaminants encountered at hazardous waste sites. The Air Force Research Laboratory previously worked with the U.S. Environmental Protection Agency (EPA) to develop a harmonized physiologically-based pharmacokinetic (PBPK) model for TCE; the model was updated by EPA for their use in their toxicological review.

A request was made for technical support from the Air Force Civil Engineer Center (AFCEC) and Mr. John Seibert at the Environment, Safety, and Occupational Health Directorate in the Office of the Assistant Secretary of Defense (Energy, Installations and Environment) (OASD EI&E) to participate in developing DoD health protective levels for TCE by participating in a joint effort through the TriService Toxicology Consortium (TSTC). This request involved the following tasks: 1) obtain the PBPK model EPA used in its *Toxicological Review of Trichloroethylene* dated September 2011 and demonstrate that the model may be validated; 2) perform a sensitivity analysis and in that assessment include an evaluation of EPA's Bayesian method for prior validation and impact of their use of the method (see Appendix A of the Toxicological Review); and 3) develop deliverables describing the methods used and the outcomes of each of these tasks. The methods used to complete these tasks and the resulting findings are presented in this report.

While the results of this work did not completely validate the model, it did point out some major issues with the model that should be addressed before the model is used. The validation figures, for the most part, were similar to those in EPA (2011), indicating that there are few differences between the acslX model created from the MCSim code presented in EPA (2011); the acslX conversion model is likely reproducing the MCSim model. This work also demonstrated that, with some exceptions, the model is not extremely sensitive to any of the model parameters. In cases where the model was extremely sensitive, the sensitivity may be due more to model instability and error than actual parameter sensitivity. Until issues in the model have been addressed, the source of these large sensitivities cannot be definitively identified. Bayesian methods used by EPA (2011) for the most part appear to be those traditionally used. There were some issues noted, but they seem minor compared to issues in the model.

2.0 INTRODUCTION

Trichloroethylene (TCE) was commonly used as a solvent by the Department of Defense (DoD), as well as at private sector facilities. Releases to the environment from its past use make TCE one of the most common contaminants encountered at hazardous waste sites. In 2011 the EPA Integrated Risk Information System (IRIS) program finalized their toxicological review for TCE (EPA, 2011). The study used for dose response for the developmental endpoint reference concentration is controversial (Johnson *et al.*, 2003). The EPA used Johnson *et al.* (2003), a rat ingestion study, to develop the reference concentration (RfC) for inhaled exposures. There is value, however, in better understanding the physiologically-based pharmacokinetic (PBPK) model used for route-to-route and inter- and intra-species extrapolation and the parameters to which the model is sensitive. AFRL previously worked with EPA to develop a harmonized PBPK model for TCE (Hack *et al.*, 2006) but it was updated by EPA for their use in their toxicological review (EPA, 2011). A more mechanistic understanding of the PBPK model will provide insight into the uncertainty associated with its use by EPA (2011) to derive a human RfC. This understanding will enhance risk communication efforts to the public and DoD personnel that may be exposed to TCE via the inhalation pathway. It will also be useful to those that may use Johnson *et al.* (2003) to determine values protective of occupational health and enable estimation of the impact that a repeat of the Johnson *et al.* (2003) study may have on the RfC.

A request was made for technical support from the Air Force Civil Engineer Center (AFCEC) and Mr. John Seibert at the Environment, Safety, and Occupational Health Directorate in the Office of the Assistant Secretary of Defense (Energy, Installations and Environment) (OASD EI&E) to participate in developing DoD health protective levels for TCE by participating in a joint effort through the TriService Toxicology Consortium (TSTC). This request involved the following tasks: 1) obtain the PBPK model EPA used in its *Toxicological Review of Trichloroethylene* dated September 2011 and demonstrate that the model may be validated; 2) perform a sensitivity analysis and in that assessment include an evaluation of EPA's Bayesian method for prior validation and impact of their use of the method (see Appendix A of the Toxicological Review); and 3) develop deliverables describing the methods used and the outcomes of each of these tasks. The methods used to complete these tasks and the resulting findings are presented below.

This effort will assist in developing DoD health protective levels for TCE. It will also identify data gaps that will reduce uncertainty in current and future protective levels.

3.0 TASK 1A: OBTAIN THE PBPK MODEL EPA USED

3.1 Methods

The *Toxicological Review of Trichloroethylene* (EPA, 2011) was downloaded from the internet. Various versions of the model are available; this report uses the September 2011 version. The report and appendices were downloaded and the links provided in the model report's Appendix A were followed to download the supplemental material. The model code was then copied from the PDF of Appendix A of EPA (2011), pasted into a text file, and reformatted for use in acslX (formerly provided by AEgis Technologies, Orlando FL). The EPA model code was formatted for MCSim (Bois, 2009).

Reformatting involved deleting unnecessary lines of code (*e.g.*, lines defining input, output, and state variables in MCSim that are not used in acslX) and some recoding to account for differences between how MCSim completes some tasks and how acslX completes them (*e.g.*, integration, code for dosing). Some variables were also renamed slightly for consistency (*e.g.*, RUrnTCA was renamed to RAUrnTCA) or to be shorter (*e.g.*, "Collect" in the variable name changed to "Coll"). Units for the constants were updated in the comments if appropriate and were added, when known, if missing in the comments.

Variables calculated in the MCSim code but not used as an output or in another calculation were deleted. These variables were carried over from previous model versions and lacked both purpose and explanation of their original definition in the current model. Deleting unused code keeps the model size, memory requirements, and required computational time to a minimum. Below is an alphabetical listing of these deleted parameters.

AUrnTCA_Sat	RUrnTCOGTCOH	VGutCtmp
AUrnTCOG_Sat	StochChlorTCE	VKidCtmp
AUrnTCOGTCOH_Sat	StochDCATCE	VLivCtmp
CDCVG_ND	StochTCEGluc	VPlasCtmp
CDCVG_NDtmp	TCAUrnSat	VRapCtmp
CDCVGmolLD	TCOGUrnSat	VRespEffCtmp
CDCVGmol0	VBldCtmp	VRespLumCtmp
MWChlor	VBodCtmp	VSlwCtmp
QRapCtmp	VBodTCOHCtmp	zAUrnTCA_Sat
RUrnNDCVC	VFatCtmp	

3.2 Potential Problems Found in Code

Several concerns with the EPA (2011) model were noted during the process of converting the code from MCSim to acslX. One potential problem with the EPA (2011) model is the lack of coding to ensure mass balance in tissue blood flows and volumes when selecting parameters values from the parameter distributions. This coding appears to be the same as was used by Bois (2000) and Hack *et al.* (2006). While unlikely, if the upper bounds (as given in the MCSim files

in the supplemental material) for all of the fractional blood flows were selected for an iteration, the sum of these fractional blood flows (QFatC, QGutC, QKidC, QLivC and QSlwC) would sum to more than 1.0. This alone would cause issues with mass balance for the flows; however, the rapidly perfused blood flow (QRap) is calculated as cardiac output (QC) minus the sum of these blood flows such that the blood flow for rapidly perfused tissues would be negative. The potential for negative values also exists for the fractional tissue volumes, although only the current human upper bounds and the human female priors could potentially result in a mass imbalance. For the project task of validating the model, this model coding issue isn't important as both the prior and posterior means do not create mass imbalances for flow or volumes.

Another concern is that the EPA (2011) model contains numerous statements that essentially reset variable values to zero if the variable value was less than 0 or a variable used in its calculation was less than 0 (*e.g.*, if ABodTCA is less than zero, the model sets CBodTCA to zero rather than ABodTCA/VBod). If the equations and model are correctly defined and mass balance is maintained, these statements should not be necessary in any model. It should also be noted that some of the venous blood concentrations leaving the tissues (*e.g.*, CVBodTCOH) are defined using the amount in the tissue and the tissue volume rather than the concentration in the tissue so while the tissue concentration is reset to essentially zero, the venous blood concentration leaving the tissue is not. The model is inconsistent in that some tissues are calculated this way and others are not. These statements were maintained in the acslX code as the tasks of this project did not involve correcting the model, and one can see in the output numerous instances of where the variable value being plotted has been reset.

Another issue is the updated respiratory metabolism code. For non-inhalation dosing, the code results in negative values for the concentration in the inhalation respiratory tract lumen (CInhResp) and the respiratory tract tissue (CResp) which, in turn, result in negative values for concentration in arterial blood (CArt) and the exhalation respiratory tract lumen (CExhResp). For some of the inhalation dosing simulations, the model also predicted unexpected drops in venous blood concentration (CVen), indicating it may also not be working as intended for inhalation dosing. It is suspected that these issues may be due to how the code separates the respiratory tract lumen into separate inhalation and exhalation pieces, but this was not further explored.

Lastly, it is worth noting that revisions to the Hack *et al.* (2006) model to create the EPA (2011) model resulted in the removal of the dichloroacetic acid (DCA) sub-model. While this does not affect the performance of the model, DCA is one of the TCE metabolites of greatest concern with regards to toxic effects; thus the removal of the DCA sub-model is viewed as a scientific shortcoming impairing the ability of the EPA (2011) model to predict TCE toxicity.

3.3 Results

The completed reformatting of the model code compiled in acslX with no errors.

4.0 TASK 1B: DEMONSTRATE THAT THE MODEL MAY BE VALIDATED

4.1 Methods

Due to the manner in which the results were presented in EPA (2011) and the fact that no manner of validation was given in the statement of work, it was determined that validation of the model would be demonstrated by reproducing Figures A-31, A-32 and A-34 as most of these data were available in the MCSim files supplied in the supplemental data. Figures A-33 and A-35 were not used as these data were not included in the MCSim file. In order to accomplish this, M files were created with the parameters used and the information from the MCSim files in the supplemental data. Prior and posterior parameter values were compiled using Tables 3-37 through 3-39 in EPA (2011) and Tables A-4, A-9, A-12, and A-15 in Appendix A of EPA (2011). M files for each study were created with the simulation settings and data presented in the MCSim files in the supplemental data. Since these MCSim files were in PDF format, the text was copied from the PDF and pasted into text files and the data blocks were reformatted as necessary. The manuscripts from which the data were obtained were compiled and used to double check dosing settings for the simulations.

All of the M files were run to generate the output for reproducing Figures A-31, A-32, and A-34. It is important to note that these reproduced figures will differ from the ones in EPA (2011) in that the lines for the simulations will be smoother for the reproductions. EPA (2011) simulations using MCSim output the endpoint values at discrete time points that matched the data collection time points. The output from the acslX runs to validate the model were continuous time-courses for the simulation period; thus, more points are plotted on the simulation lines in the reproduced figures. The reproduced figures use the same axis-scale limits as EPA (2011) figures to the extent possible; however, limits were altered as necessary to ensure all of the data and the simulation are shown. The figures here are in the same order as those they reproduce from EPA (2011).

4.2 Concerns in Validating the Model

It was difficult to compile the prior and posterior parameter values. The parameters listed in Tables 3-37 thru 3-39 in EPA (2011) are not necessarily the parameters needed for input into the model (*e.g.*, QP is given in the table but the model calculates QP using QC and VPR; VPR is not given in the table) or were not in the correct units for input into the model (*e.g.*, QC in L/hour is given in the table but the model uses QCC in L/hour/kg$^{0.75}$). Not all of the parameter values are given in Table A-4 in Appendix A of EPA (2011). Also, several parameter names in Tables A-4, A-9, A-12, and A-15 are preceded by "ln" which would imply the values given are the natural log of the parameter value; however, the values given appear to have already been transformed.

Therefore it was assumed that all of the values in Tables A-4, A-9, A-12, and A-15 were natural-space values and needed no transformations prior to use. Spreadsheets were created for mouse, rat, and human with available values from Tables 3-37 through 3-39, Tables A-4, A-9, A-12, and A-15, and those given in the model code itself. From these sources, not all prior values agreed

and not all posterior values agreed. In general, all prior values were taken from the model code. Exceptions are:

- Mouse and rat values for the following are from Table 3-37: DRespC, FracLungSysC, FracOtherC, kAD, kAS, kASTCA, kBileC, kDCVGC, kEHRC, kKidBioactC, KMClara, kMetTCAC, kMetTCOHC, KMGluc, KMTCOH, kNATC, kTSD, PEffDCVG, VMaxGlucC, VMaxTCOHC
- Mouse values for the following are from Table 3-37: FracKidDCVCC, kASTCOH, kTD
- Rat value for kAsTCOH is from Table A-12
- Human values for the following are from Table 3-37: ClGluc, ClTCOH, DRespC, FracOtherC, FracLungSysC, kAD, kAS, kASTCA, kASTCOH, kBileC, kDCVGC, kEHRC, kKidBioactC, KMClara, kMetTCOHC, kMetTCAC, KMGluc, KMTCOH, kNATC, kTSD, PEffDCVG

The posterior values used are calculated using the priors (see above) and the posterior changes given in Tables A-9, A-12, and A-15 in Appendix A of EPA (2011). Simulations in the presented figures use the posterior values. Figures A-31, A-32, and A-34 in Appendix A of EPA (2011) state that the posterior subject-specific parameters were used, but those parameters were not given. Tables 1 through 4 show the values that were found.

An additional issue encountered in creating the M files was the truncation of some of the data lines in the PDF of the MCSim files. These missing points had to be digitized from the original papers. The individual data points for alveolar breath concentration (CAlvPPM) in Chiu *et al.* (2007) (in the supplemental data) were difficult to distinguish so these data were digitized from the relevant boxes in Figure A-34. The inhaled concentrations for the Chiu *et al.* (2007) data sets were also truncated. As these data were not found, the available values were used. For the remaining time of exposure, the last concentration value was used.

There were discrepancies in trying to align the reproduced figures for human data from Kimmerle and Eben (1973a) with those in Appendix A of EPA (2011). The simulations for the reproduced figures were run in the same order as the data in the MCSim file from the supplemental data of EPA (2011). In the Kimmerle and Eben (1973a) paper, there are single exposure data for four females (one exposed to 40 ppm and three exposed to 44 ppm) and four males (three exposed to 40 ppm and one exposed to 44 ppm); however, in the MCSim file in the supplemental data, there are only data for three males (two at 40 ppm and one at 44 ppm). From the figures in Appendix A of EPA (2011), there are sets of figures for four females (one at 40 ppm and three at 44 ppm) and four males (three at 40 ppm and one at 44 ppm). The data in the plots from Appendix A of EPA (2011) for subject #24 look to be the same data as for subject #22 and don't match the data in the MCSim file for the remaining female exposed to 44 ppm. Based on the data, the next three figures from Appendix A of EPA (2011) look to be shifted from the data in the MCSim file. The data in the figure in Appendix A of EPA (2011) for subject #25 looks to be the data from the MCSim file that is labeled as being for a female with a single exposure to 44 ppm but the label for the figure says it is for a male with a single exposure to 40 ppm. It appears that perhaps a data set is missing from the MCSim file and that some of the

figures in Appendix A of EPA (2011) were mislabeled. For comparison purposes, the figures presented here are altered to match up with those in Appendix A of EPA (2011).

Table 1. Mouse Parameters

Parameter	Baseline[A]	Prior[B]	Posterior Changes			Reported Posterior[B]
			Fractional Increase[C]	Absolute Value[C]	Calculated Posterior[D]	
BW	0.03	--	--		0.03	--
QCC	11.6	11.6	1.237		14.3	13.9
VPR	2.5	2.5	0.8076		2.0	2.1
DRespC	--	0.00813		1.214	1.214	1.2
QFatC	0.07	0.07	1.034		0.072	0.072
QGutC	0.141	0.14	1.183		0.17	0.16
QKidC	0.091	0.092	0.995		0.091	0.091
QLivC	0.02	0.02	1.035		0.021	0.021
QSlwC	0.217	0.22	0.9828		0.21	0.21
VBldC	0.049	0.049	0.9916		0.049	0.048
VFatC	0.07	0.071	1.329		0.093	0.089
VGutC	0.049	0.049	0.9871		0.048	0.048
VKidC	0.017	0.017	1.001		0.017	0.017
VLivC	0.055	0.054	0.8035		0.044	0.047
VRapC	0.1	0.1	0.997		0.0997	0.0990
VRespLumC	0.004667	0.0047	0.9995		0.0047	0.0047
VRespC	0.0007	0.0007	1		0.0007	0.0007
VPerfC	0.8897	0.8897	--		0.8897	0.8897
FracPlas	0.52	0.53	0.8707		0.45	0.46
PB	15	15	0.9259		14	14
PFat	36	36	0.9828		35	36
PGut	1.9	1.9	0.805		1.5	1.5
PKid	2.1	2.2	1.277		2.7	2.6
PLiv	1.7	1.7	1.297		2.2	2.2
PRap	1.9	1.8	0.9529		1.8	1.8
PResp	2.6	2.7	0.9918		2.6	2.5
PSlw	2.4	2.4	0.92		2.2	2.2
PRBCPlasTCA	0.5	0.5	2.495		1.2	1.2
PBodTCAC	0.88	1.01	0.8816		0.78	0.79
PLivTCAC	1.18	1.45	0.8003		0.94	1
PBodTCOH	1.11	1.1	0.8025		0.89	0.89
PLivTCOH	1.3	1.3	1.526		1.98	1.9
PBodTCOG	1.11	0.95	0.4241		0.47	0.48
PLivTCOG	1.3	1.3	1.013		1.3	1.3
PEffDCVG	--	1.25		0.9807	1.0	1
BMaxkDC	0.88	1.15	1.25		1.1	1.5

Parameter	Baseline[A]	Prior[B]	Posterior Changes			Reported Posterior[B]
			Fractional Increase[C]	Absolute Value[C]	Calculated Posterior[D]	
kDissoc	107	100	1.214		130	130
kAS	--	1.7		1.711	1.7	1.7
kTSD	--	1.4		5.187	5.2	4.5
kAD	--	1.2		0.2665	0.27	0.27
kTD	--	0.1		0.1002	0.1	0.1
kASTCA	--	0.63		3.986	4.0	4
kASTCOH	--	0.75		0.7308	0.73	0.73
VMaxC	2700	2407	0.6693		1807	1773
KM	36	34	0.07148		2.6	2.7
Cl	--	--	--			--
FracTCAC	0.32	0.18	0.4875		0.16	0.15
FracOtherC	--	0.75		0.02384	0.024	0.025
VMaxDCVGC	300	2284	1.517		455	426
KMDCVGC	*	*	--		*	*
ClDCVG	1.53	9.14	0.1794		0.27	0.19
VMaxKidDCVGC	60	667	1.424		85	53
KMKidDCVGC	*	*	--		*	*
ClKidDCVG	0.34	4.44	0.827		0.28	0.33
VMaxLungLiv	0.0701021 (0.07)	0.062	2.903		0.203	0.17
KMClara	--	1.5		0.01123	0.011	0.011
FracLungSysC	--	0.52		3.304	3.3	3.50
VMaxTCOHC	--	0.89		1.645	1.6	1.7
KMTCOH	--	1.4		0.9594	0.96	0.92
ClTCOH	--	--	--			--
VMaxGlucC	--	1.53		65.59	66	64
KMGluc	--	1.8		31.16	31	30
ClGluc	--	--	--			--
kMetTCOHC	--	0.079		3.629	3.6	3.7
kUrnTCAC	0.6	0.83	0.1126		0.07	0.07
kMetTCAC	--	0.05		0.6175	0.62	0.62
kBileC	--	0.13		0.9954	1.0	0.1
kEHRC	--	0.087		0.01553	0.016	0.016
kUrnTCOGC	0.6	0.8	7.874		4.7	4.8
kDCVGC	--	0.1		0.2266	0.23	0.34
FracKidDCVCC	--	1.9		1.931	1.9	1.9
kNATC	--	0.12		0.1175	0.12	0.15
kKidBioactC	--	0.075		0.07506	0.075	0.096

Notes: All values are from EPA (2011) unless noted otherwise. [A]Value source is model code and value in parentheses is from Table A-4 when different from model code; [B]Value source is Table 3-37; [C]Value source is Table A-9; [D]Based on Table A-9 and Baseline Value; --Value not found; *Calculated in model; Blue colored number doesn't agree with value from Table A-4/Model Code; Red colored number doesn't agree with value using Table A-9 and priors.

Table 2. Rat Parameters

Parameter	Baseline[A]	Prior[B]	Posterior Changes			Reported Posterior[B]
			Fractional Increase[C]	Absolute Value[C]	Calculated Posterior[D]	
BW	0.3	--	--		0.3	--
QCC	13.3	13	1.195		16	15
VPR	1.9	1.9	0.6304		1.20	1.2
DRespC	--	0.99		2.765	2.765	2.8
QFatC	0.07	0.071	1.167		0.082	0.081
QGutC	0.153	0.15	1.154		0.18	0.17
QKidC	0.141	0.14	1.002		0.14	0.14
QLivC	0.021	0.021	1.029		0.022	0.022
QSlwC	0.336	0.33	0.9086		0.31	0.31
VBldC	0.074	0.073	1.002		0.074	0.074
VFatC	0.07	0.069	0.9728		0.068	0.069
VGutC	0.032	0.032	0.9826		0.031	0.032
VKidC	0.007	0.0069	0.999		0.007	0.007
VLivC	0.034	0.034	0.9608		0.033	0.033
VRapC	0.088	0.087	0.9929		0.087	0.088
VRespLumC	0.0046667 (0.004667)	0.0046	1.001		0.004672	0.0047
VRespC	0.0005	0.0005	0.999		0.0005	0.0005
VPerfC	0.8995	0.8995	--		0.8995	0.8995
FracPlas	0.53	0.53	1.037		0.55	0.54
PB	22	22	0.8551		19	19
PFat	27	27	1.17		32	31
PGut	1.4	1.3	0.8197		1.1	1.1
PKid	1.3	1.3	0.9209		1.2	1.2
PLiv	1.5	1.5	1.046		1.6	1.6
PRap	1.3	1.3	1.021		1.3	1.3
PResp	1	0.97	0.993		1.0	1
PSlw	0.58	0.57	1.258		0.73	0.73
PRBCPlasTCA	0.5	0.53	0.9763		0.49	0.52
PBodTCAC	0.88	0.9	1.136		1.000	0.97
PLivTCAC	1.18	1.1	1.283		1.5	1.4
PBodTCOH	1.11	1	0.9454		1.0	1.1
PLivTCOH	1.3	1.3	0.926		1.2	1.2
PBodTCOG	1.11	0.48	1.968		2.2	1.6
PLivTCOG	1.3	1.3	7.484		10	10
PEffDCVG	--	1		--	1.0	1
BMaxkDC	1.22	1.2	0.9654		1.2	1.1
kDissoc	275	270	1.01		278	280
kAS	--	0.73		2.474	2.5	2.5
kTSD	--	1.4		3.747	3.7	3.2

Parameter	Baseline[A]	Prior[B]	Posterior Changes			Reported Posterior[B]
			Fractional Increase[C]	Absolute Value[C]	Calculated Posterior[D]	
kAD	--	0.96		0.1731	0.17	0.17
kTD	--	0	--		0	--
kASTCA	--	0.83		1.513	1.5	1.4
kASTCOH	--	--		0.6896	0.69	0.69
VMaxC	600	569	0.8948		537	535
KM	21	18	0.0239		0.50	0.74
Cl	--	--	--		--	--
FracTCAC	0.32	0.26	0.2348		0.075	0.069
FracOtherC	--	0.028		0.344	0.34	0.41
VMaxDCVGC	66	196	7.749		511	586
KMDCVGC	*	*	--		*	*
ClDCVG	0.25	0.13	0.3556		0.089	0.093
VMaxKidDCVGC	6	18	0.2089		1.3	1.1
KMKidDCVGC	*	*	--		*	*
ClKidDCVG	0.026	0.039	184		4.8	4.6
VMaxLungLiv	0.0143 (0.0144)	0.034	2.673		0.038	0.032
KMClara	--	0.016		0.02563	0.026	0.025
FracLungSysC	--	4.6		2.729	2.7	2.7
VMaxTCOHC	--	1.9		1.832	1.8	1.8
KMTCOH	--	1		22.09	22	19
ClTCOH	--	--	--		--	--
VMaxGlucC	--	67		28.72	29	27
KMGluc	--	31		6.579	6.6	6.3
ClGluc	--	--	--		--	--
kMetTCOHC	--	3.1		2.354	2.4	2.2
kUrnTCAC	0.522	0.074	0.07112		0.037	0.037
kMetTCAC	--	0.56		0.3554	0.36	0.35
kBileC	--	1		8.7	9	10
kEHRC	--	0.0096		1.396	1.4	1.3
kUrnTCOGC	0.522	4.6	20.65		11	17
kDCVGC	--	22202	--		22202	22202
FracKidDCVCC	1 (--)	--	--		1	1
kNATC	--	0.11		0.002035	0.00204	0.0022
kKidBioactC	--	0.09		0.006618	0.0066	0.0068

Notes: All values are from EPA (2011) unless noted otherwise. [A]Value source is model code and value in parentheses is from Table A-4 when different from model code; [B]Value source is Table 3-37; [C]Value source is Table A-9; [D]Based on Table A-9 and Baseline Value; --Value not found; *Calculated in model; Blue colored number doesn't agree with value from Table A-4/Model Code; Red colored number doesn't agree with value using Table A-9 and priors.

Table 3. Human Female Parameters

Parameter	Baseline[A]	Prior[B]	Posterior Changes			Reported Posterior[B]
			Fractional Increase[C]	Absolute Value[C]	Calculated Posterior[D]	
BW	60	--	--		60	--
QCC	16	16	0.837		13.4	13.9
VPR	0.96	0.97	1.519		1.46	2.1
DRespC	--	1.47		0.626	0.63	1.2
QFatC	0.085	0.051	0.7781		0.066	0.072
QGutC	0.21	0.19	0.7917		0.17	0.16
QKidC	0.17 (0.085)	0.19	1.007		0.171	0.19
QLivC	0.065	0.063	0.5099		0.033	0.021
QSlwC	0.17	0.22	0.7261		0.12	0.21
VBldC	0.068	0.077	1.013		0.069	0.078
VFatC	0.317	0.19	0.788		0.25	0.16
VGutC	0.022	0.02	1		0.022	0.02
VKidC	0.0046	0.0043	0.9965		0.0046	0.0043
VLivC	0.023	0.026	1.043		0.024	0.026
VRapC	0.093	0.087	0.9959		0.093	0.088
VRespLumC	0.002386	0.0024	1.003		0.0024	0.0024
VRespC	0.00018	0.00018	1		0.00018	0.00018
VPerfC	0.85778	0.856	--		0.85778	0.856
FracPlas	0.615 (0.065)	0.57	1.001		0.62	0.56
PB	9.5	9.6	0.9704		9.2	9.2
PFat	67	68	0.8498		57	57
PGut	2.6	2.6	1.095		2.8	2.9
PKid	1.6	1.6	0.9993		1.6	1.6
PLiv	4.1	4	0.9907		4.1	4.1
PRap	2.6	2.6	0.93		2.4	2.4
PResp	1.3	1.3	1.018		1.3	1.3
PSlw	2.1	2.1	1.157		2.4	2.3
PRBCPlasTCA	0.5	0.49	0.3223		0.2	0.2
PBodTCAC	0.52	0.58	1.194		0.62	0.68
PLivTCAC	0.66	0.76	1.202		0.79	0.85
PBodTCOH	0.91	0.89	1.703		1.5	1.5
PLivTCOH	0.59	0.58	1.069		0.63	0.63
PBodTCOG	0.91	0.67	0.7264		0.66	0.72
PLivTCOG	0.59	1.8	6.671		3.9	3.1
PEffDCVG	--	1.24		0.01007	0.01007	0.012
BMaxkDC	4.62	4.6	0.8806		4.1	4.1
kDissoc	182	180	0.9932		181	180
kAS	--	1.4	--		1.4	1.4
kTSD	--	1.4	--		1.4	1.4

Parameter	Baseline[A]	Prior[B]	Posterior Changes			Reported Posterior[B]
			Fractional Increase[C]	Absolute Value[C]	Calculated Posterior[D]	
kAD	--	0.75	--		0.75	0.75
kTD	0 (--)	--	--		0	--
kASTCA	--	0.58		4.511	4.5	3
kASTCOH	--	0.49		8.262	8.3	7.6
VMaxC	255	236	0.3759		96	104
KM	*	*	--		*	*
Cl	66	64	12.64		834	580
FracTCAC	0.32	0.28	0.1315		0.042	0.041
FracOtherC	--	0.14		0.1186	0.12	0.12
VMaxDCVGC	*	*	--		*	*
KMDCVGC	2.9	3.1	1.213		3.5	3.6
ClDCVG	19	18	2.786		53	52
VMaxKidDCVGC	*	*	--		*	*
KMKidDCVGC	2.7	2.7	0.2802		0.76	0.76
ClKidDCVG	230	271	0.04538		10.4	9.2
VMaxLungLiv	0.0273 (0.0138)	0.058	3.772		0.103	0.095
KMClara	--	0.019		0.2726	0.27	0.31
FracLungSysC	--	3		24.08	24	24
VMaxTCOHC	--	*	--		*	*
KMTCOH	--	5		2.221	2.2	2.2
ClTCOH	--	0.35		0.1767	0.18	0.17
VMaxGlucC	--	*	--		*	*
KMGluc	--	10		133.4	133	130
ClGluc	--	3		0.2796	0.28	0.29
kMetTCOHC	--	2.47		0.7546	0.75	0.72
kUrnTCAC	0.108	0.011	0.04565		0.0049	0.0048
kMetTCAC	--	0.55		0.2812	0.28	0.28
kBileC	--	3.47		6.855	6.86	7.23
kEHRC	--	0.21		0.1561	0.16	0.15
kUrnTCOGC	0.108	1.6	15.78		1.7	1.4
kDCVGC	--	0.127		7.123	7.12	7.23
FracKidDCVCC	--	--	--	--	--	--
kNATC	--	0.0025		0.000316	0.00032	0.00029
kKidBioactC	--	0.0064		0.06516	0.065	0.067

Notes: All values are from EPA (2011) unless noted otherwise. [A]Value source is model code and value in parentheses is from Table A-4 when different from model code; [B]Value source is Table 3-37; [C]Value source is Table A-9; [D]Based on Table A-9 and Baseline Value; --Value not found; *Calculated in model; Blue colored number doesn't agree with value from Table A-4/Model Code; Red colored number doesn't agree with value using Table A-9 and priors.

Table 4. Human Male Parameters

Parameter	Baseline[A]	Prior[B]	Posterior Changes			Reported Posterior[B]
			Fractional Increase[C]	Absolute Value[C]	Calculated Posterior[D]	
BW	70	--	--		70	--
QCC	16	16	0.837		13.4	13.9
VPR	0.96	0.97	1.519		1.46	2.1
DRespC	--	1.47		0.626	0.63	1.2
QFatC	0.05	0.051	0.7781		0.04	0.072
QGutC	0.19	0.19	0.7917		0.15	0.16
QKidC	0.19 (0.05)	0.19	1.007		0.191	0.19
QLivC	0.065	0.063	0.5099		0.033	0.021
QSlwC	0.22	0.22	0.7261		0.16	0.21
VBldC	0.077	0.077	1.013		0.078	0.078
VFatC	0.199	0.19	0.788		0.16	0.16
VGutC	0.02	0.02	1		0.020	0.02
VKidC	0.0043	0.0043	0.9965		0.0043	0.0043
VLivC	0.025	0.026	1.043		0.026	0.026
VRapC	0.088	0.087	0.9959		0.088	0.088
VRespLumC	0.002386	0.0024	1.003		0.0024	0.0024
VRespC	0.00018	0.00018	1		0.00018	0.00018
VPerfC	0.856	0.856	--		0.856	0.856
FracPlas	0.567 (0.065)	0.57	1.001		0.57	0.56
PB	9.5	9.6	0.9704		9.2	9.2
PFat	67	68	0.8498		57	57
PGut	2.6	2.6	1.095		2.8	2.9
PKid	1.6	1.6	0.9993		1.6	1.6
PLiv	4.1	4	0.9907		4.1	4.1
PRap	2.6	2.6	0.93		2.4	2.4
PResp	1.3	1.3	1.018		1.3	1.3
PSlw	2.1	2.1	1.157		2.4	2.3
PRBCPlasTCA	0.5	0.49	0.3223		0.2	0.2
PBodTCAC	0.52	0.58	1.194		0.62	0.68
PLivTCAC	0.66	0.76	1.202		0.79	0.85
PBodTCOH	0.91	0.89	1.703		1.5	1.5
PLivTCOH	0.59	0.58	1.069		0.63	0.63
PBodTCOG	0.91	0.67	0.7264		0.66	0.72
PLivTCOG	0.59	1.8	6.671		3.9	3.1
PEffDCVG	--	1.24		0.01007	0.01007	0.012
BMaxkDC	4.62	4.6	0.8806		4.1	4.1
kDissoc	182	180	0.9932		181	180
kAS	--	1.4	--		1.4	1.4
kTSD	--	1.4	--		1.4	1.4

Parameter	Baseline[A]	Prior[B]	Posterior Changes			Reported Posterior[B]
			Fractional Increase[C]	Absolute Value[C]	Calculated Posterior[D]	
kAD	--	0.75	--		0.75	0.75
kTD	0 (--)	--	--		0	--
kASTCA	--	0.58		4.511	4.5	3
kASTCOH	--	0.49		8.262	8.3	7.6
VMaxC	255	236	0.3759		96	104
KM	*	*	--		*	*
Cl	66	64	12.64		834	580
FracTCAC	0.32	0.28	0.1315		0.042	0.041
FracOtherC	--	0.14		0.1186	0.12	0.12
VMaxDCVGC	*	*	--		*	*
KMDCVGC	2.9	3.1	1.213		3.5	3.6
ClDCVG	19	18	2.786		53	52
VMaxKidDCVGC	*	*	--		*	*
KMKidDCVGC	2.7	2.7	0.2802		0.76	0.76
ClKidDCVG	230	271	0.04538		10.4	9.2
VMaxLungLiv	0.0253 (0.0128)	0.058	3.772		0.095	0.095
KMClara	--	0.019		0.2726	0.27	0.31
FracLungSysC	--	3		24.08	24	24
VMaxTCOHC	--	*	--		*	*
KMTCOH	--	5		2.221	2.2	2.2
ClTCOH	--	0.35		0.1767	0.18	0.17
VMaxGlucC	--	*	--		*	*
KMGluc	--	10		133.4	133	130
ClGluc	--	3		0.2796	0.28	0.29
kMetTCOHC	--	2.47		0.7546	0.75	0.72
kUrnTCAC	0.108	0.011	0.04565		0.0049	0.0048
kMetTCAC	--	0.55		0.2812	0.28	0.28
kBileC	--	3.47		6.855	6.86	7.23
kEHRC	--	0.21		0.1561	0.16	0.15
kUrnTCOGC	0.108	1.6	15.78		1.7	1.4
kDCVGC	--	0.127		7.123	7.12	7.23
FracKidDCVCC	--	--	--	--	--	--
kNATC	--	0.0025		0.000316	0.00032	0.00029
kKidBioactC	--	0.0064		0.06516	0.065	0.067

Notes: All values are from EPA (2011) unless noted otherwise. [A]Value source is model code and value in parentheses is from Table A-4 when different from model code; [B]Value source is Table 3-37; [C]Value source is Table A-9; [D]Based on Table A-9 and Baseline Value; --Value not found; *Calculated in model; Blue colored number doesn't agree with value from Table A-4/Model Code; Red colored number doesn't agree with value using Table A-9 and priors.

The Chiu *et al.* (2007) data in the figures from EPA (2011) Appendix A for TCOG and TCA in urine are labeled as being the amount collected rather than amount excreted. The data in the paper are labeled as cumulative excreted amount. In the MCSim file, these data appear to have been treated as amount collected data rather than amount excreted; however, as the values are consistently increasing, these data appear to be cumulative amount excreted. Given the discrepancy, the validation figures below show simulations for amount excreted rather than amount collected to be consistent with the labeling of the data Chiu *et al.* (2007). Also, the time points for these data in the MCSim file do not seem to correspond to the time points for the data presented in the paper. There also appear to be more time points for these data in the paper and the paper's supplemental material than are included in the MCSim file. As the lines in the MCSim file do not appear to have been truncated, it is unclear why they differ.

4.3 Results

Reproduced figures for the mouse, rat and human are shown in the attached Appendices A, B, and C, respectively. The model code is given in Appendix D. M files to generate these figures for mouse, rat and human are given in Appendices E, F, and G, respectively, with the corresponding data presented in Appendices H, I, and J. Some of the reproduced figures appear to match the figures in Appendix A of EPA (2011) quite well, while others do not match and some are quite a bit off. However, even for those figures that match poorly, the shape of the curves are similar thus supporting that the discrepancies are more likely due to parameterization issues than model conversion issues. As noted above, the figures in Appendix A of EPA (2011) use the posterior subject-specific parameters whereas the reproduced figures use the population posterior means. Posterior subject-specific parameters can vary quite a bit from population posteriors; however, these values were not given in the report.

5.0 TASK 2A: PERFORM A SENSITIVITY ANALYSIS

5.1 Methods

Sensitivity analyses were conducted for the mouse, rat, and human at the same TCE doses and exposure scenarios as used by EPA (2011) for their sensitivity analyses. Only three of the dosemetrics used by EPA (2011) for their sensitivity analyses were included in the MCSim code in the supplemental material. These values were area-under-the curve calculations for arterial blood concentrations of TCE (CArt) and TCOH (CTCOH) and liver concentration of free TCA (CLivTCA). Mouse and rat simulations were to simulate inhalation (100 and 600 ppm) exposure for 7 hours per day, 5 days per week or to simulate oral gavage (300 and 1000 mg/kg/day) exposure 5 days per week. Most of the rodent simulations were run for 10 weeks. Weekly "averages" for the dosemetrics were calculated for mouse and rat as the final value minus the value at the end of the previous week. By the end of the simulations using mean posterior parameter values, simulations for CArt, CTCOH and CLivTCA had reached periodicity. The model simulations demonstrated some instability in predictions for rat inhalation exposure; thus

these simulations were run for only one week. These exceptions are described in more detail below.

Separate simulations were run for male and females; simulations for both were run for continuous exposure to 0.001 ppm or 0.001 mg/kg/day. All human simulations were run for 100 weeks and daily “averages” were calculated. Simulations for CArt, CTCOH and CLivTCA using mean posterior parameter values had reached a sort of periodicity (discussed further below). Daily “averages” were calculated as the final value minus the value at the end of the previous day.

Calculations for the sensitivity analysis used the central difference method with increases and decreases for the posterior parameter values of 5 percent (*i.e.*, overall change in input parameter of 10 percent). Sensitivity coefficients were calculated using the equation from EPA (2011). Coefficients were also calculated as the ratio of fractional change in output to fractional change in input (see below for further detail).

5.2 Concerns in Conducting the Sensitivity Analysis

Of the ten endpoints used by the EPA, only three were in the MCSim code included in the supplemental data. Definitions or descriptions on how the remaining endpoints were calculated could not be found in any of the EPA documentation; therefore, the analyses presented here were only conducted on three endpoints. The endpoints that could not be located are:

- For mouse, rat and human: FracMetab, FracOxMetab, FracMetGSH, FracMetLiv1, FracMetLivOther, FracMetLng
- For rat and human only: FracBioactKid

EPA (2011) stated that they simulated continuous oral dosing to 0.001 mg/kg/day, but they did not state whether they simulated this exposure as a drinking water dose or as a continuous gavage dose. It was assumed that simulations were run as drinking water doses. Running the model to simulate a continuous oral gavage dose resulted in predictions for CArt, CTCOH, and CLivTCA that were the same as those for simulating continuous drinking water exposure.

When checking the simulations for the various exposures for periodicity, it was noted that the first simulation in a modeling session predicted extremely high values for CArt and CLivTCA as though something was not being initialized correctly. Subsequent simulations resulted in values closer to those expected. Parameter settings in the initial section were double checked for definitions and order of equations. It was also checked that parameters calculated in the Dynamic section were sorted appropriately and were not used in the Derivative section (*i.e.*, they were parameters for output only). It is unclear whether this issue is related to model problems discussed above or is due to some other problem.

Rat simulations for CTCOH for inhalation exposure demonstrated some unexpected downward spikes, but predictions were still all above zero. These spikes occurred at random times across

the entire time period such that just running the simulations for a shorter time period did not avoid them. It is unclear what impact these spikes had on dosemetric predictions.

In addition to these spikes, the simulations for inhalation exposure did not finish for changes in some of the parameters: body weight (BW), fractional volume of respiratory tissue (VRespC), liver/blood partition coefficient (PLiv), capacity for hepatic TCE oxidation (VMaxC), affinity for hepatic TCE oxidation (KMC) and affinity for tracheo-bronchial TCE oxidation (KMClara).

- For 100 ppm: Simulations were achieved up to about 536 hours (a little over three weeks) for BW, about 896 hours (a little over five weeks) for VRespC, and about 440 hours (a little over two weeks) for KMClara. The simulations for CArt, CTCOH, and CLivTCA looked to be the same after one week as for subsequent weeks so the simulations for changes in these parameters were stopped at 168 hours.
- For 600 ppm: Simulations would not run past about 13.5 hours for BW, 13.4 hours for VRespC, and 109.0 hours for PLiv and KMC. Therefore, a weekly dosemetric could not be calculated for this dose and changes in these parameters. Simulations were achieved up to about 229 hours (a little over one week) for VMaxC and about 421 hours (a little over two weeks) for KMClara. The simulations for changes in these parameters were stopped at 168 hours.

Human simulations for CArt, CTCOH, and CLivTCA following inhalation exposure did not look as expected. The simulations approach a steady state level, but the level line is jagged and shows repeated increases and decreases (Figure 1 inset), resulting in the apparent thick line (Figure 1 main graph). For continuous oral exposure, the human simulations for females begin with an unusual behavior but appears to "level" out to a behavior similar to that seen for inhalation exposure (see Figures 2 through 4). The plots of the area-under-the-curve for these endpoints result in straight lines after the initial time frame (Figures 5 through 7). Male simulations, however, have a truly odd behavior throughout the entire simulation (Figures 8 through 10) and appear to indicate discontinuous exposure that repeats approximately every 800 or 900 hours even though the input rate into the gut is steady (Figure 11). The parameter settings between male and female, however, only differ in some physiological parameters that should not be causing this behavior. The plots of the area-under-the-curve of the endpoints (Figures 12 through 14) reiterate this behavior.

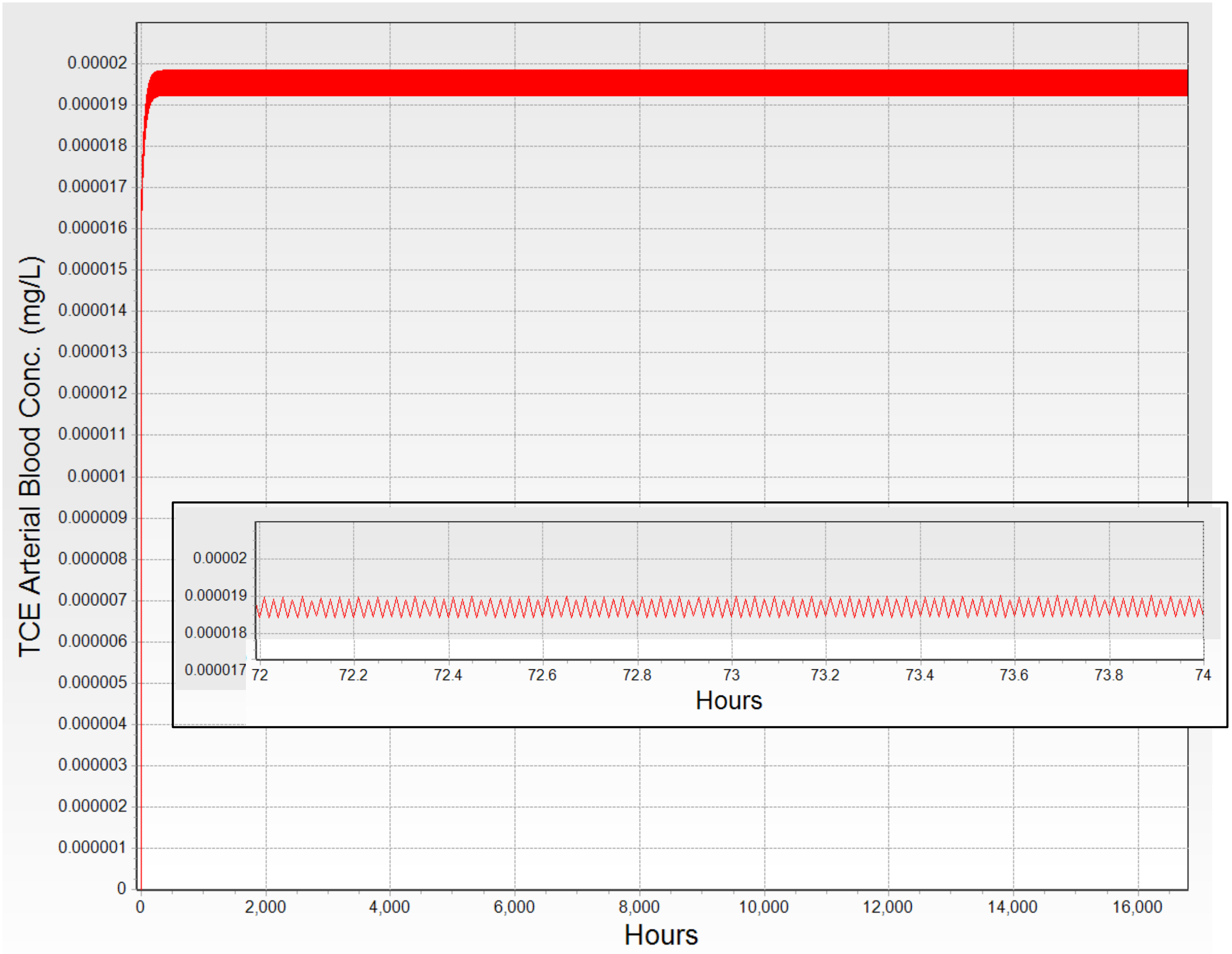

Figure 1. TCE Arterial Blood Concentration in Females Following Continuous Inhalation Exposure to 0.001 ppm. Inset is the same simulation on a shorter time scale to better demonstrate behavior.

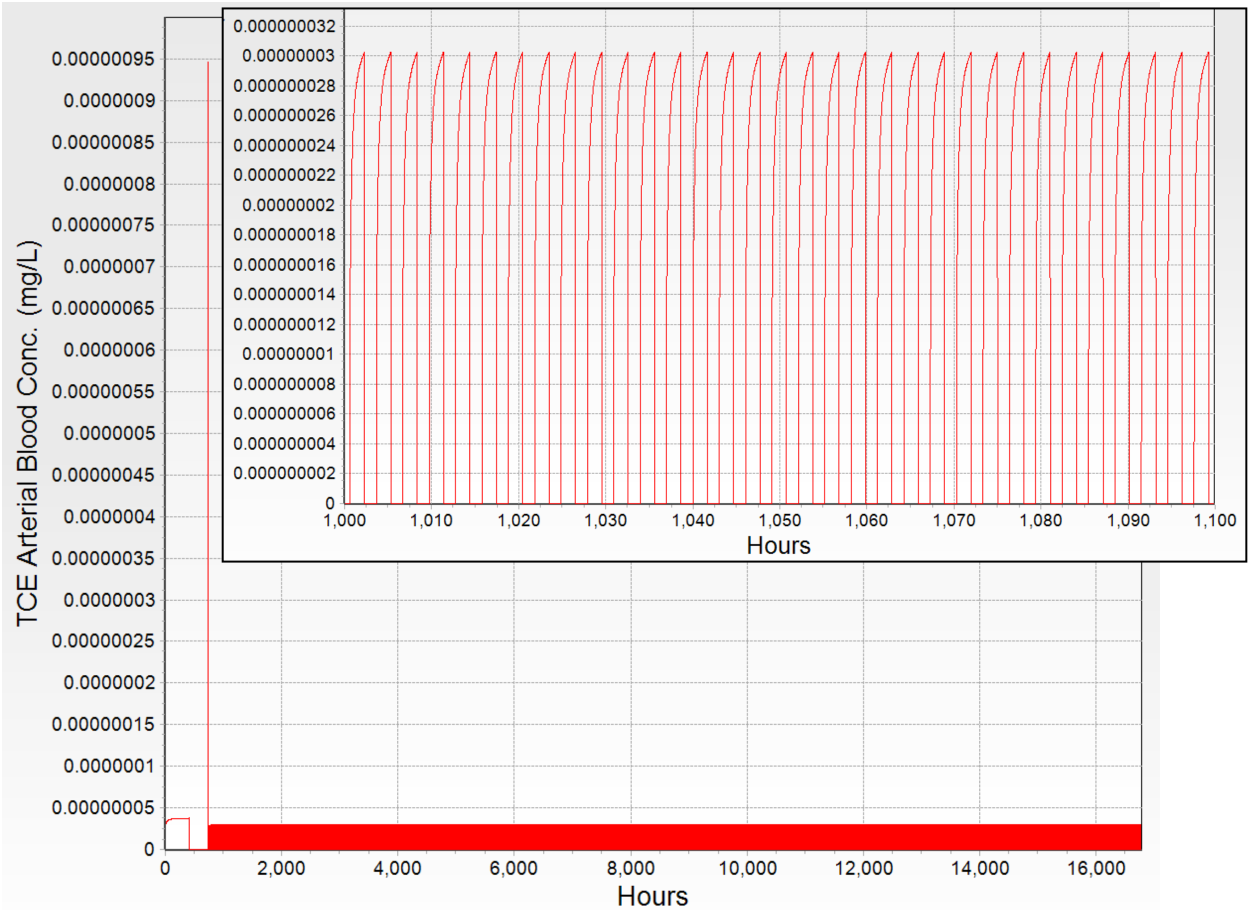

Figure 2. TCE Arterial Blood Concentration in Females Following Continuous Drinking Water Exposure to 0.001 mg/kg/day. Inset is the same simulation on a shorter time scale to better demonstrate behavior.

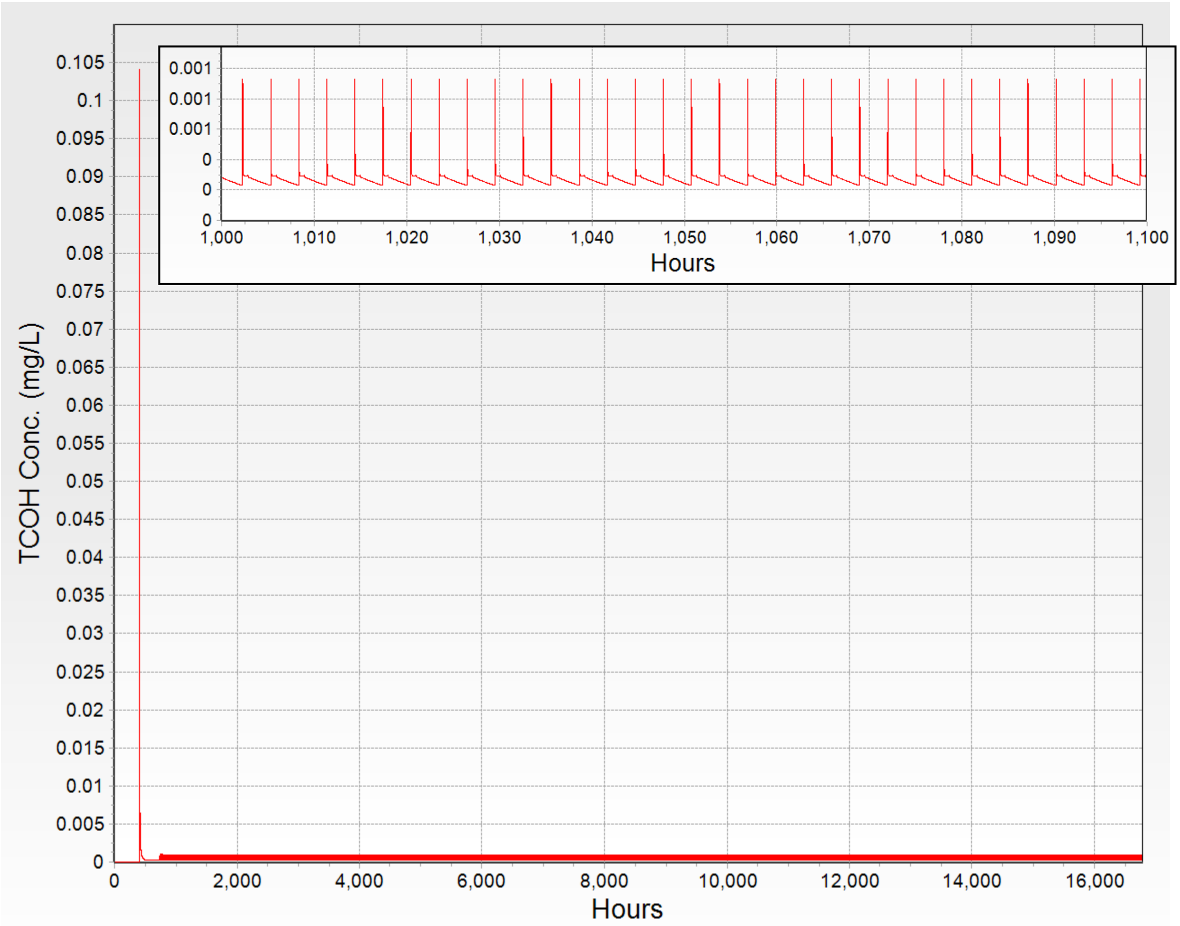

Figure 3. TCOH Concentration in Females Following Continuous Drinking Water Exposure to 0.001 mg/kg/day. Inset is the same simulation on a shorter time scale to better demonstrate behavior.

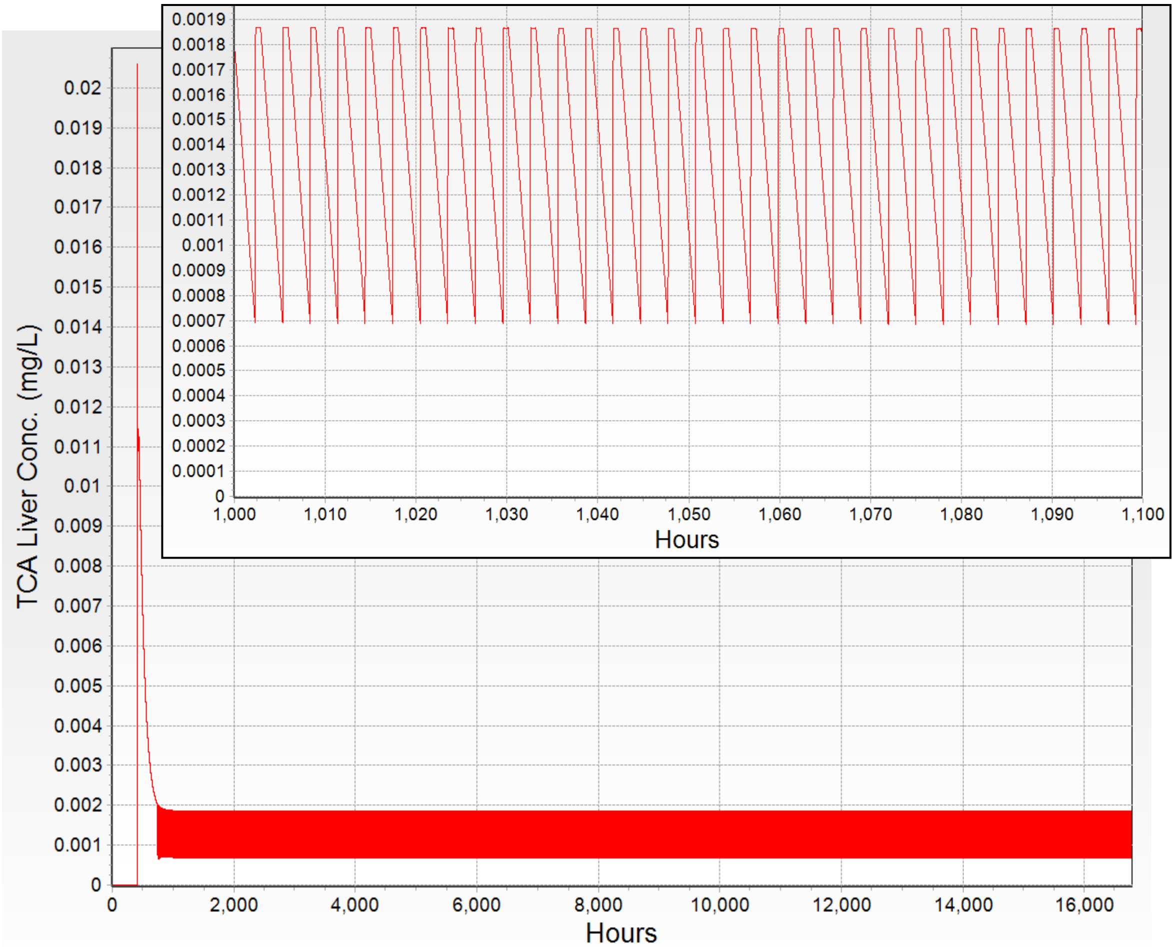

Figure 4. TCA Liver Concentration in Females Following Continuous Drinking Water Exposure to 0.001 mg/kg/day. Inset is the same simulation on a shorter time scale to better demonstrate behavior.

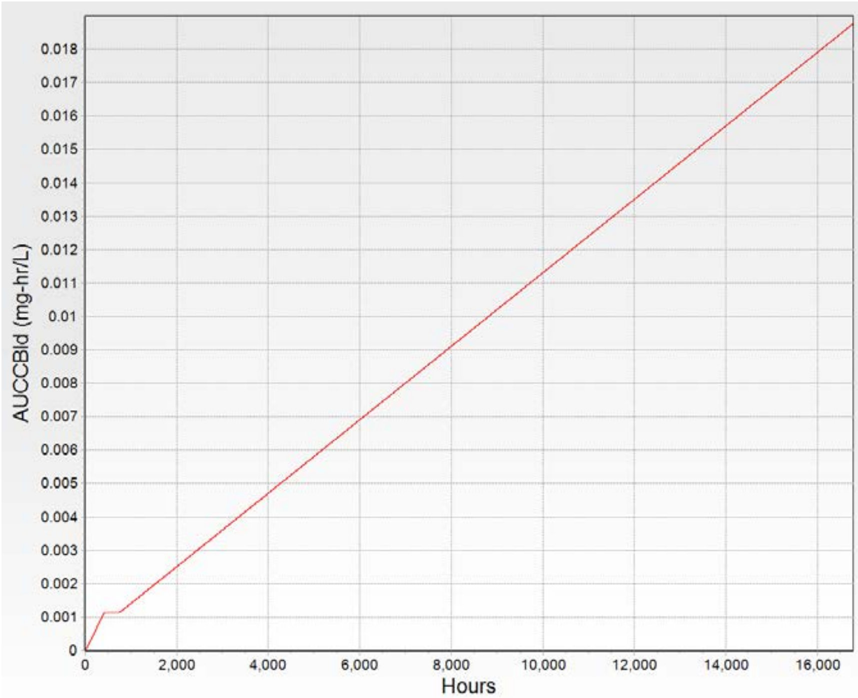

Figure 5. Area Under the Curve for TCE Arterial Blood Concentration for Females Following Continuous Drinking Water Exposure to 0.001 mg/kg/day

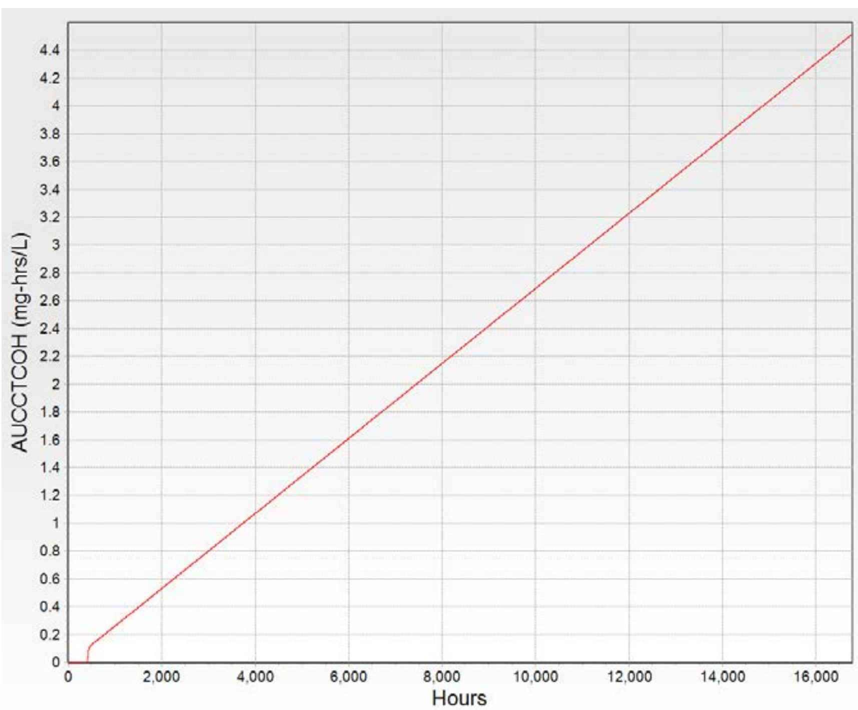

Figure 6. Area Under the Curve for TCOH Concentration for Females Following Continuous Drinking Water Exposure to 0.001 mg/kg/day

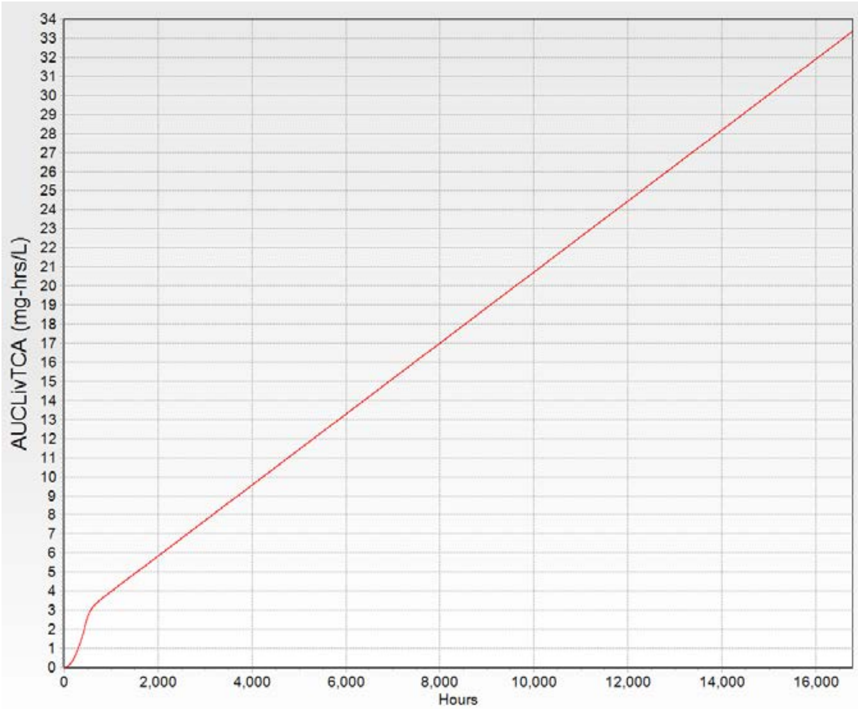

Figure 7. Area Under the Curve for TCA Liver Concentration for Females Following Continuous Drinking Water Exposure to 0.001 mg/kg/day

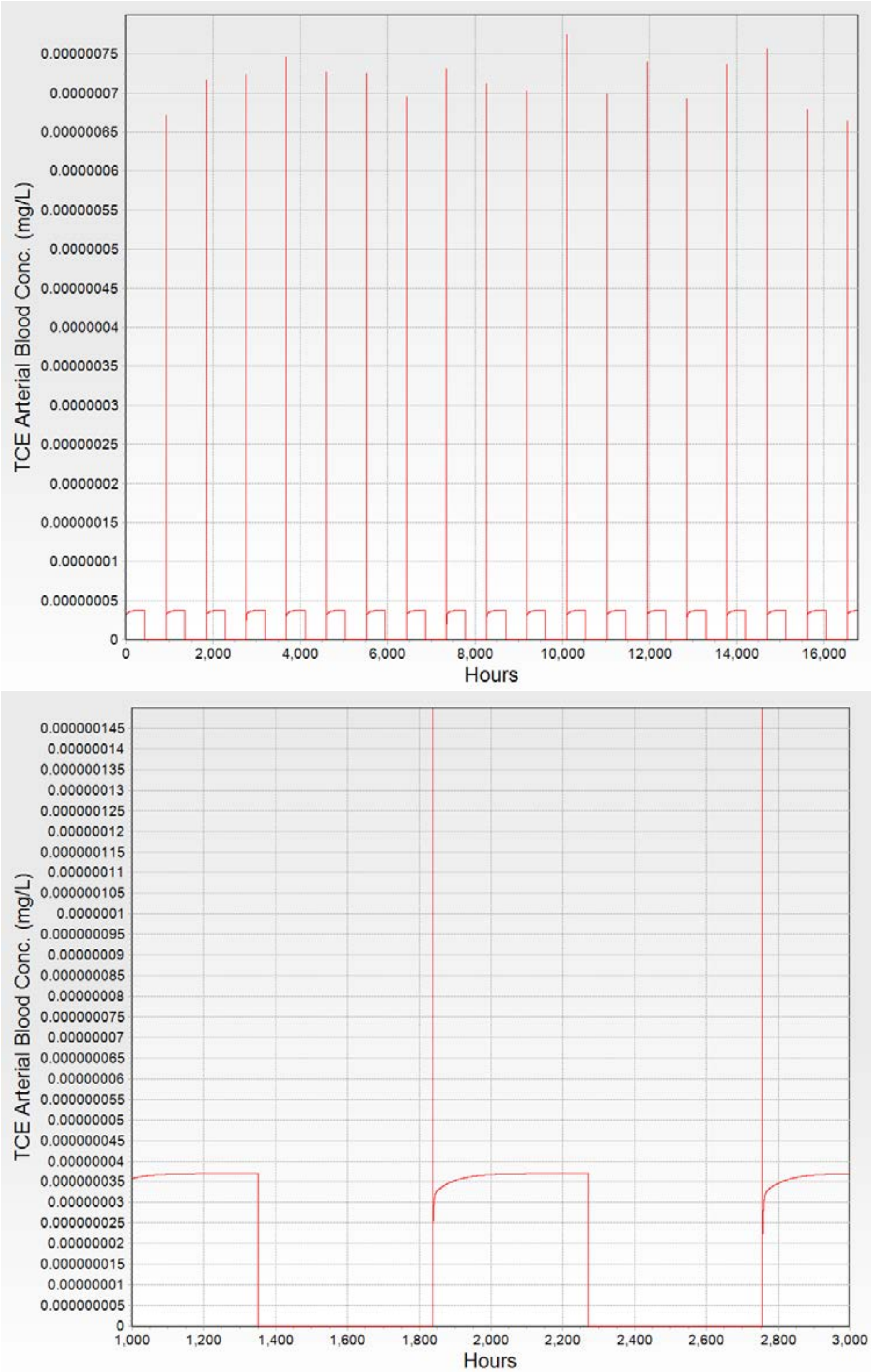

Figure 8. TCE Arterial Blood Concentration in Males Following Continuous Drinking Water Exposure to 0.001 mg/kg/day. Bottom figure is the same simulation on a shorter time scale to better demonstrate behavior.

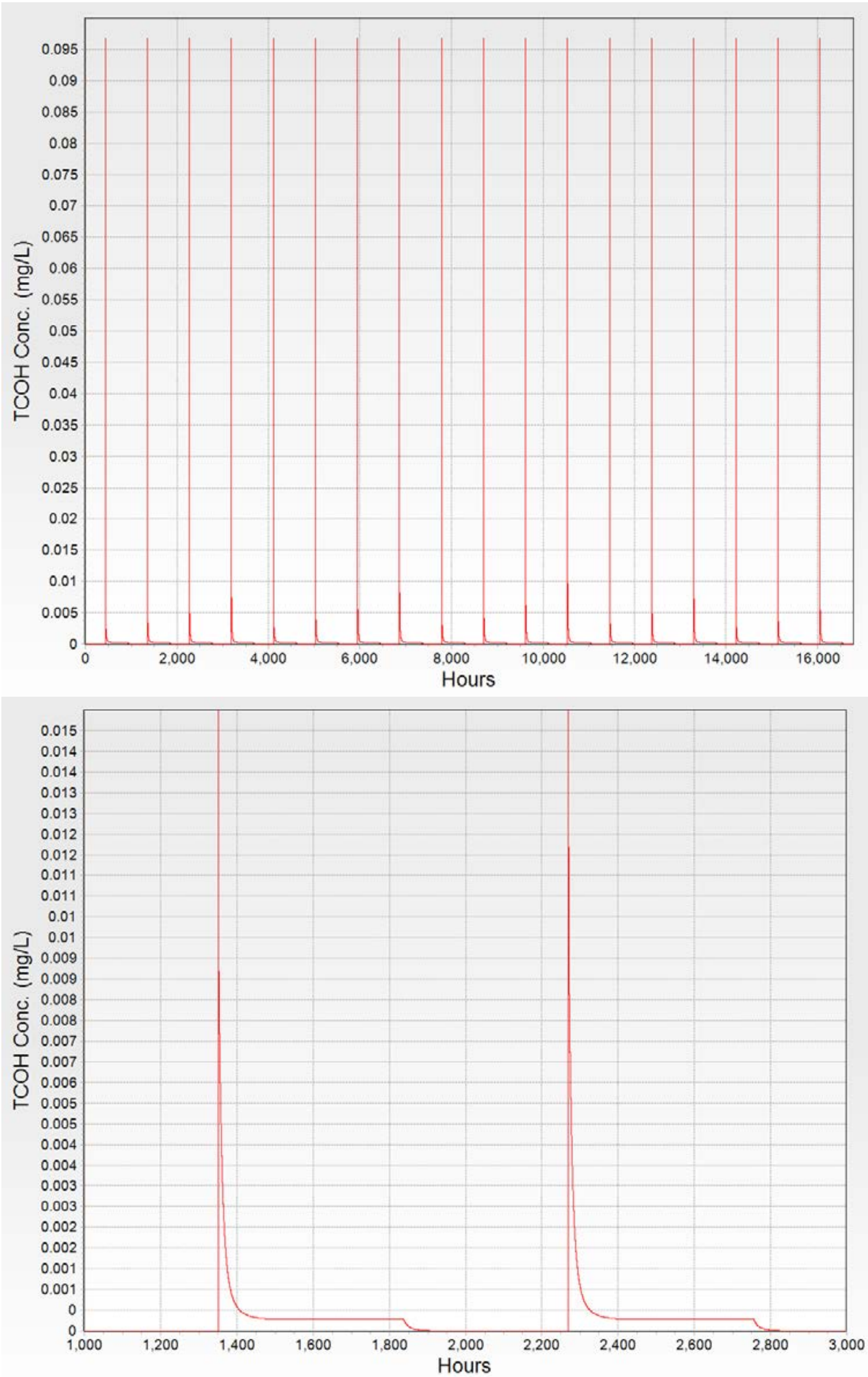

Figure 9. TCOH Concentration in Males Following Continuous Drinking Water Exposure to 0.001 mg/kg/day. Bottom figure is the same simulation on a shorter time scale to better demonstrate behavior.

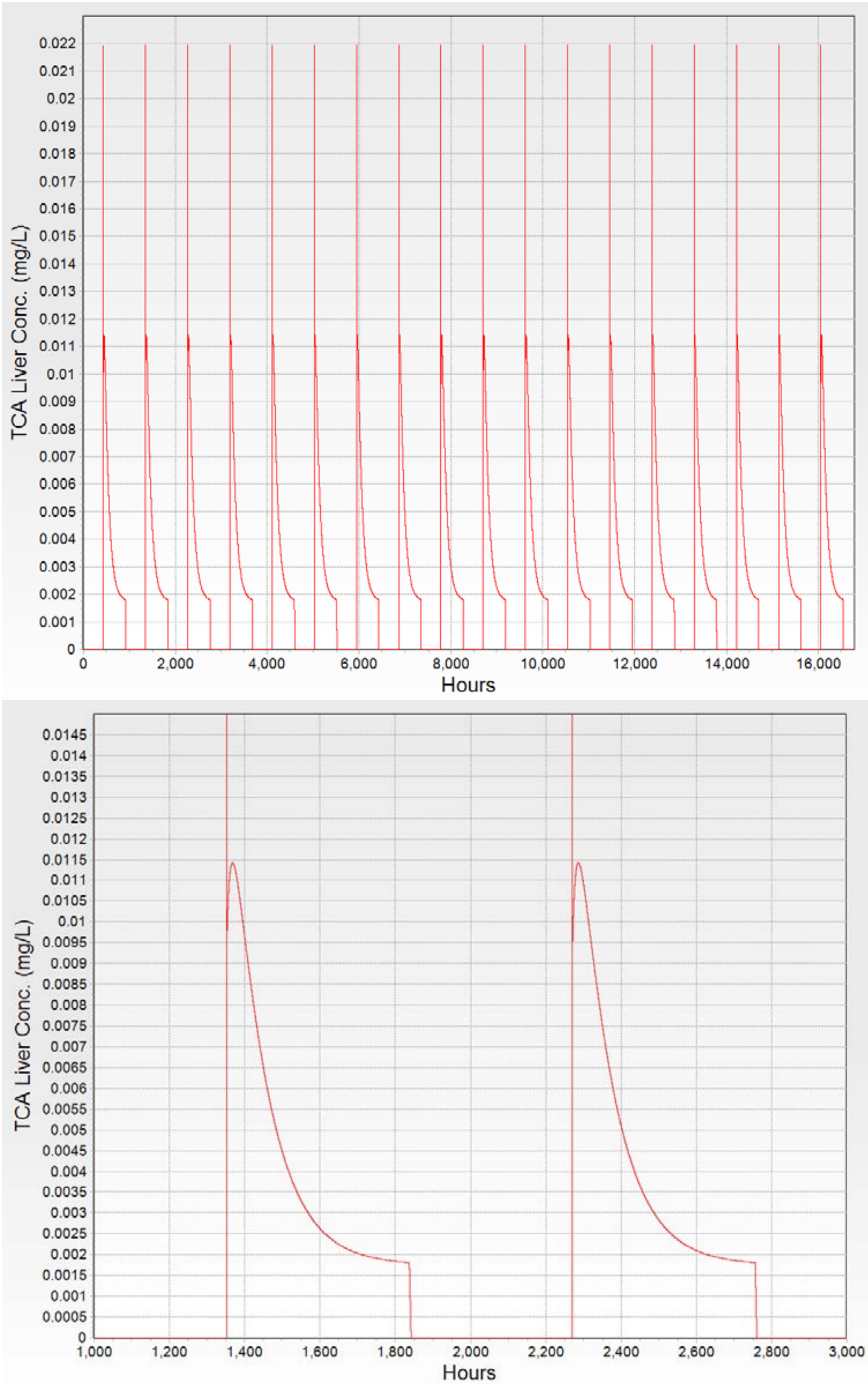

Figure 10. TCA Liver Concentration in Males Following Continuous Drinking Water Exposure to 0.001 mg/kg/day. Bottom figure is the same simulation on a shorter time scale to better demonstrate behavior.

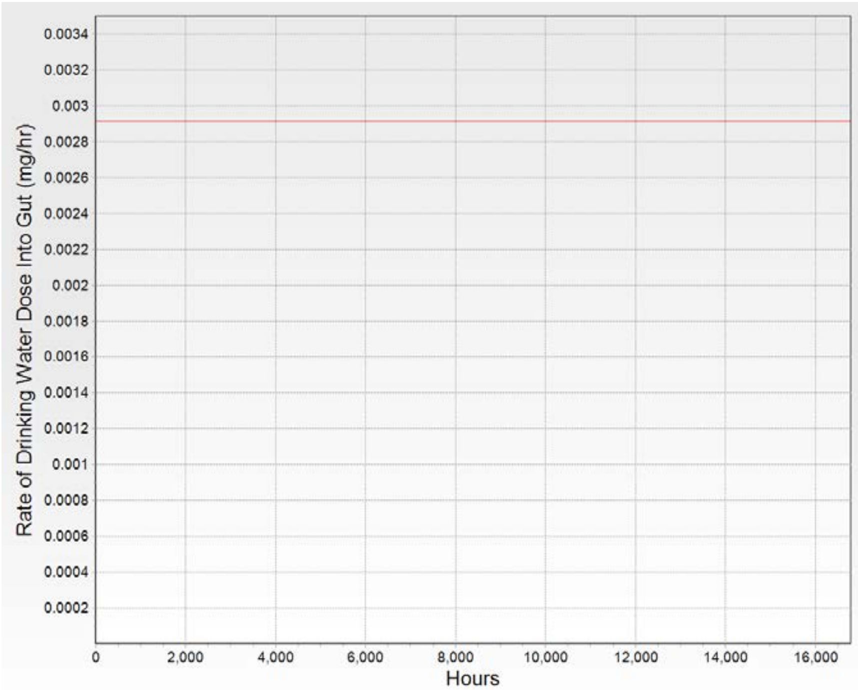

Figure 11. Rate of Input of Drinking Water Dose into Gut for Males Following Continuous Drinking Water Exposure to 0.001 mg/kg/day

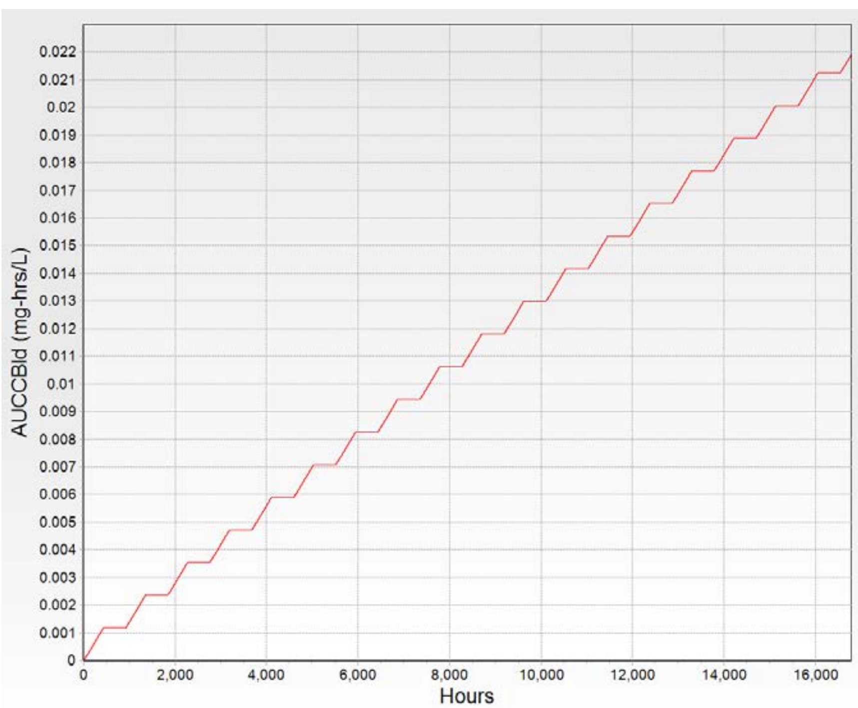

Figure 12. Area Under the Curve for TCE Arterial Blood Concentration for Males Following Continuous Drinking Water Exposure to 0.001 mg/kg/day

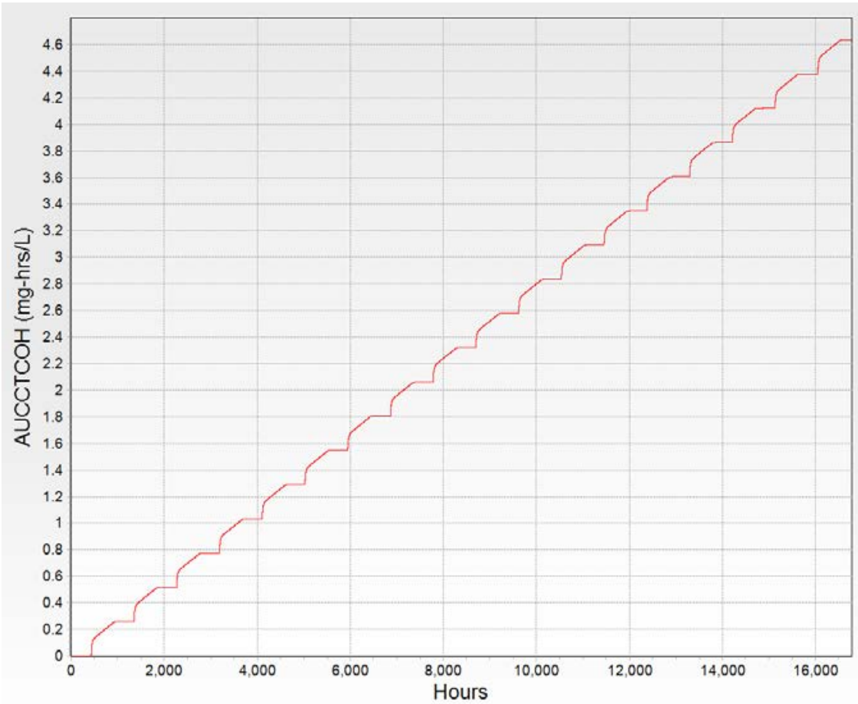

Figure 13. Area Under the Curve for TCOH Concentration for Males Following Continuous Drinking Water Exposure to 0.001 mg/kg/day

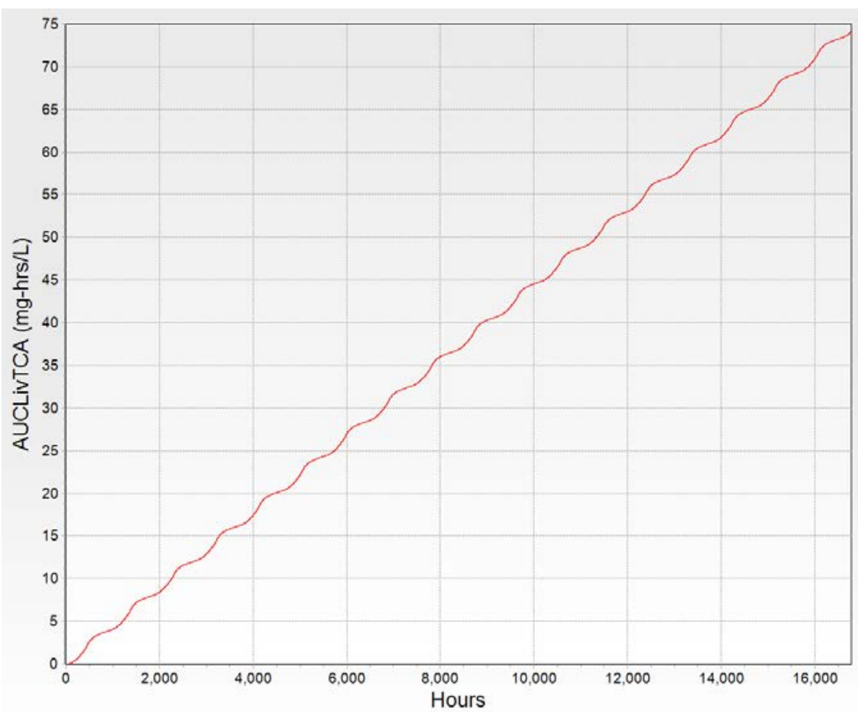

Figure 14. Area Under the Curve for TCA Liver Concentration for Males Following Continuous Drinking Water Exposure to 0.001 mg/kg/day

The equation used to calculate the sensitivity coefficients (SC) is given below. This equation normalizes the sensitivity coefficient to both the output and input parameters so that it is unitless (Kohn, 2002).

$$SC = \frac{\left(f(\theta_+) - f(\theta_-)\right)}{f(\theta_-)} \div \frac{(\theta_+ - \theta_-)}{\theta_-} = \frac{\left(f(\theta_+) - f(\theta_-)\right)}{f(\theta_-)} * \frac{\theta_-}{(\theta_+ - \theta_-)}$$

where θ_- is the baseline value minus 5 percent, θ_+ is the baseline value plus 5 percent, $f(\theta_-)$ is the response variable value resulting from an input parameter value of θ_-, and $f(\theta_+)$ is the response variable resulting from an input parameter value of θ_+. EPA (2011) used a variation of this equation to calculate their sensitivity coefficients. Since the fractional change in the input parameter is always 10 percent, that term in the equation was replaced with 10 percent or 0.1.

$$SC = \frac{\left(f(\theta_+) - f(\theta_-)\right)}{f(\theta_-)} \div 0.1 = \frac{\left(f(\theta_+) - f(\theta_-)\right)}{f(\theta_-)} * 10$$

Next, $f(\theta_-)$ in the denominator was replaced with (½ x { $f(\theta_+) + f(\theta_-)$}). So the EPA (2011) equation becomes

$$SC = \frac{\left(f(\theta_+) - f(\theta_-)\right)}{f(\theta_-)} * 10 = 10 * \frac{\left(f(\theta_+) - f(\theta_-)\right)}{\left(\frac{1}{2} * \left(f(\theta_+) + f(\theta_-)\right)\right)}$$

Given the slight difference in equations, sensitivity coefficients were calculated using both equations for comparison.

5.3 Results

The resulting sensitivity coefficients using both equations are shown in Figures 15 through 26. M files to generate these figures for mouse, rat and human are given in Appendices K, L, and M, respectively, with additional M files presented in Appendix N. Note that the figures only show sensitivity coefficients for parameters that are valid for the given dose route and that do not have coefficients of zero for all endpoints for the given route. Given that there appear to be some issues with the model code, these coefficients may be more representative of model error rather than model sensitivity. However, the M files for running the sensitivity analyses should require very little if any changes with respect to any model modifications such that rerunning the sensitivity analyses with a modified model should be fairly straight forward.

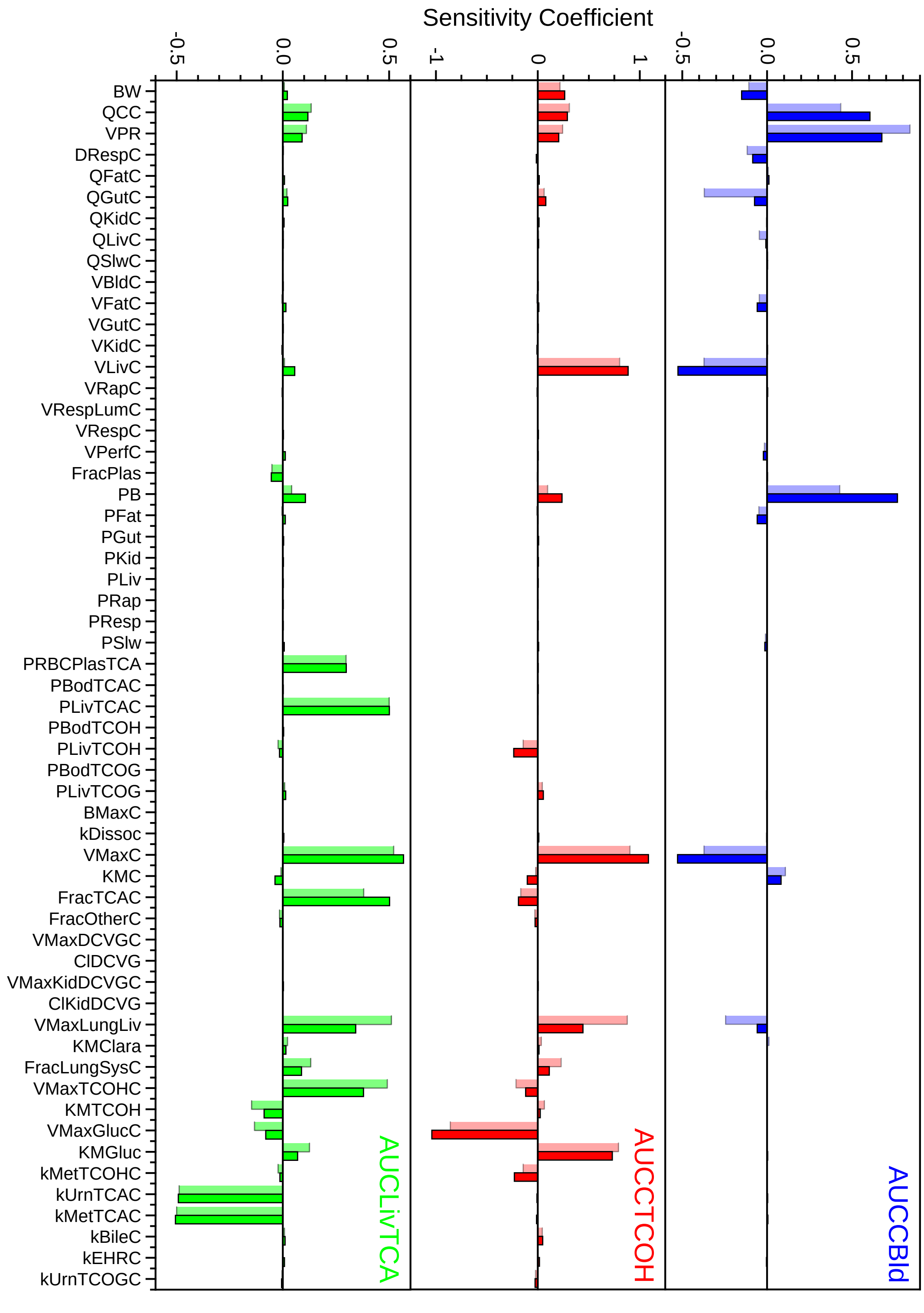

Figure 15. Sensitivity Coefficients for Mouse Following Inhalation Exposure. Exposure was 100 (light bars) or 600 ppm (dark bars) for 7 hours/day, 5 days/week for 10 weeks. Sensitivity coefficients were calculated using equation in EPA (2011).

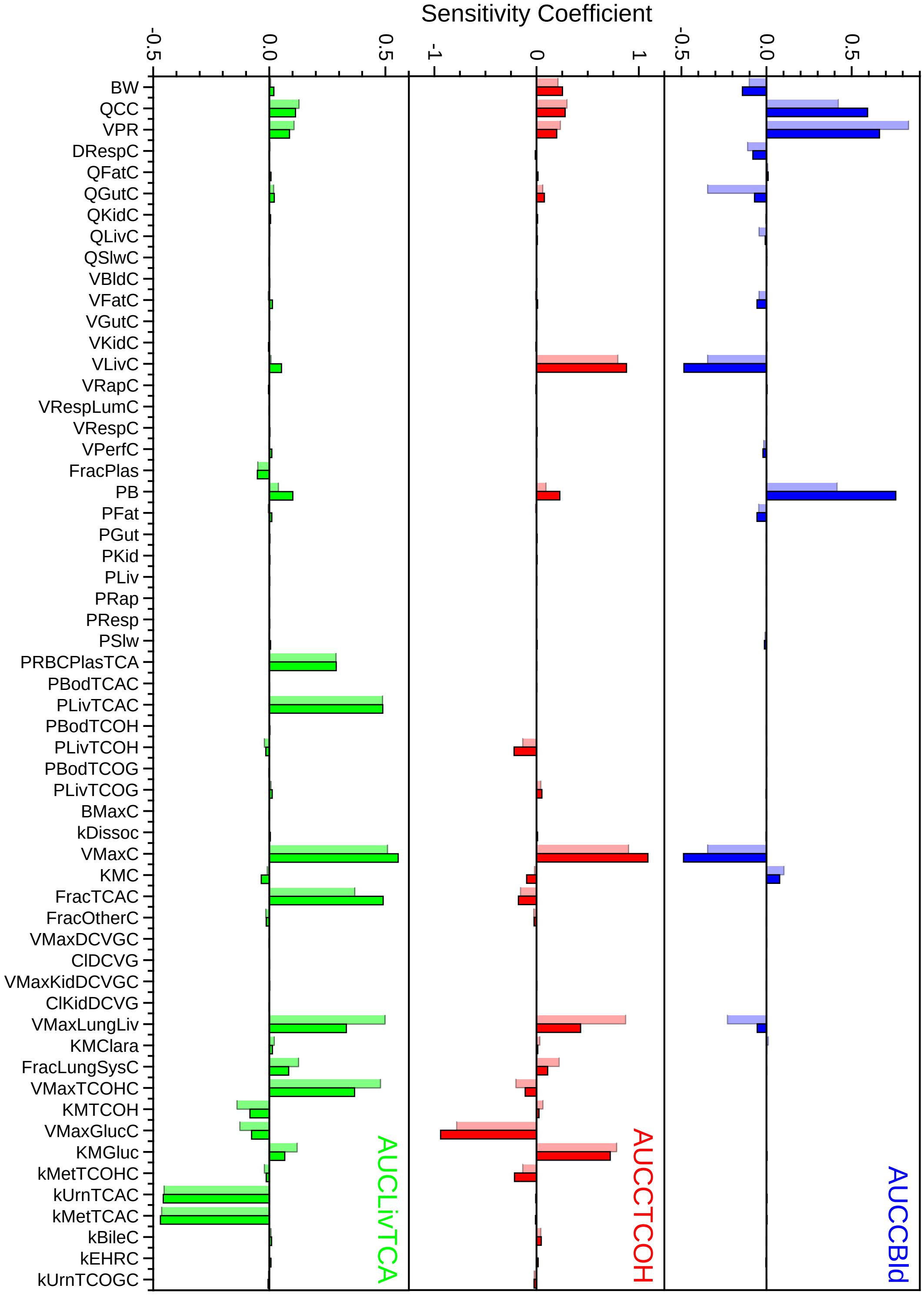

Figure 16. Sensitivity Coefficients for Mouse Following Inhalation Exposure. Exposure was 100 (light bars) or 600 ppm (dark bars) for 7 hours/day, 5 days/week for 10 weeks. Sensitivity coefficients were calculated as fraction change in output per fraction change in input.

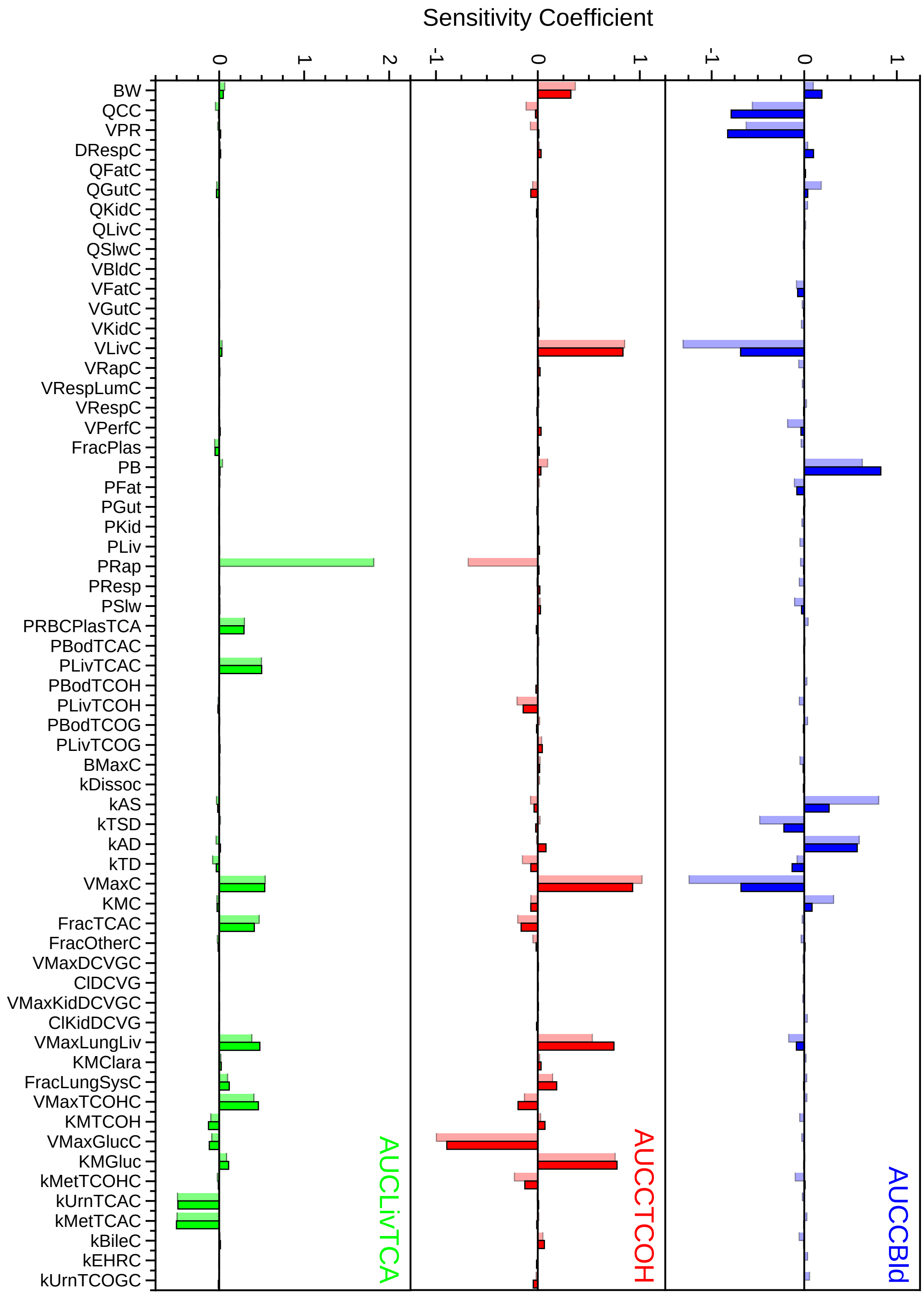

Figure 17. Sensitivity Coefficients for Mouse Following Gavage Exposure. Exposure was 300 (light bars) or 1,000 mg/kg-day (dark bars) for 5 days/week for 10 weeks. Sensitivity coefficients were calculated using equation in EPA (2011).

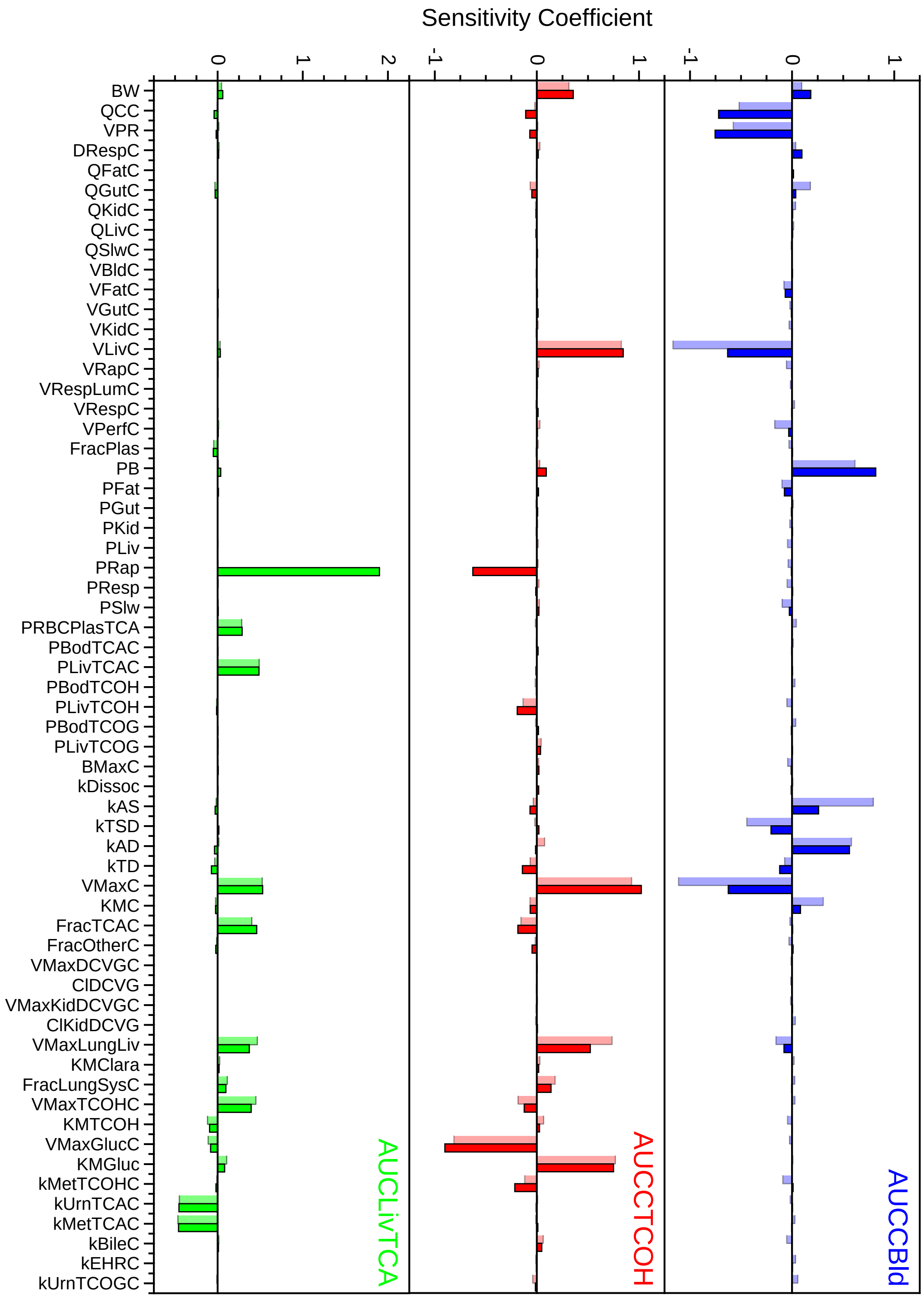

Figure 18. Sensitivity Coefficients for Mouse Following Gavage Exposure. Exposure was 300 (light bars) or 1,000 mg/kg-day (dark bars) for 5 days/week for 10 weeks. Sensitivity coefficients were calculated as fraction change in output per fraction change in input.

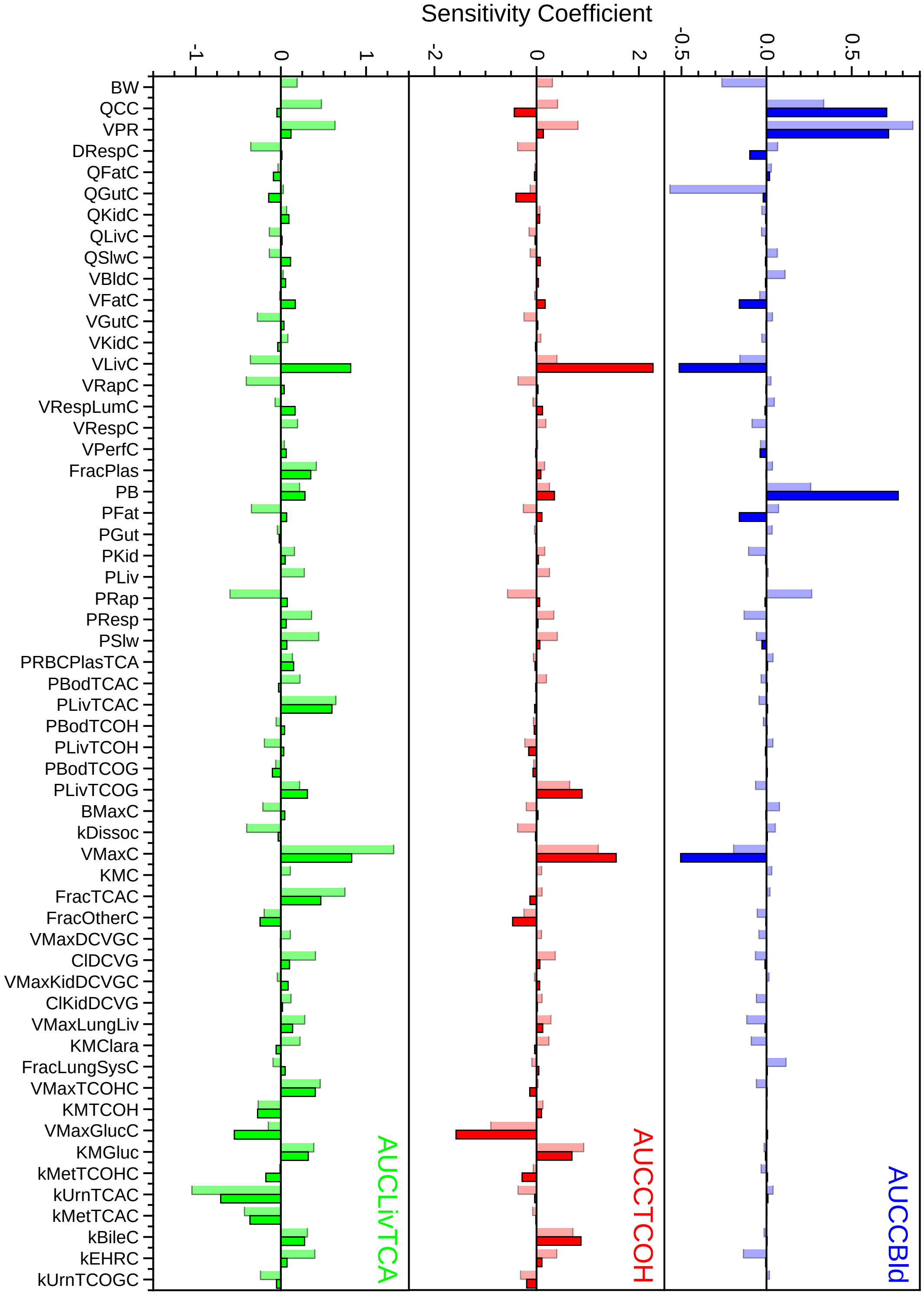

Figure 19. Sensitivity Coefficients for Rat Following Inhalation Exposure. Exposure was 100 (light bars) or 600 ppm (dark bars) for 7 hours/day, 5 days/week for 10 weeks. Sensitivity coefficients were calculated using equation in EPA (2011).

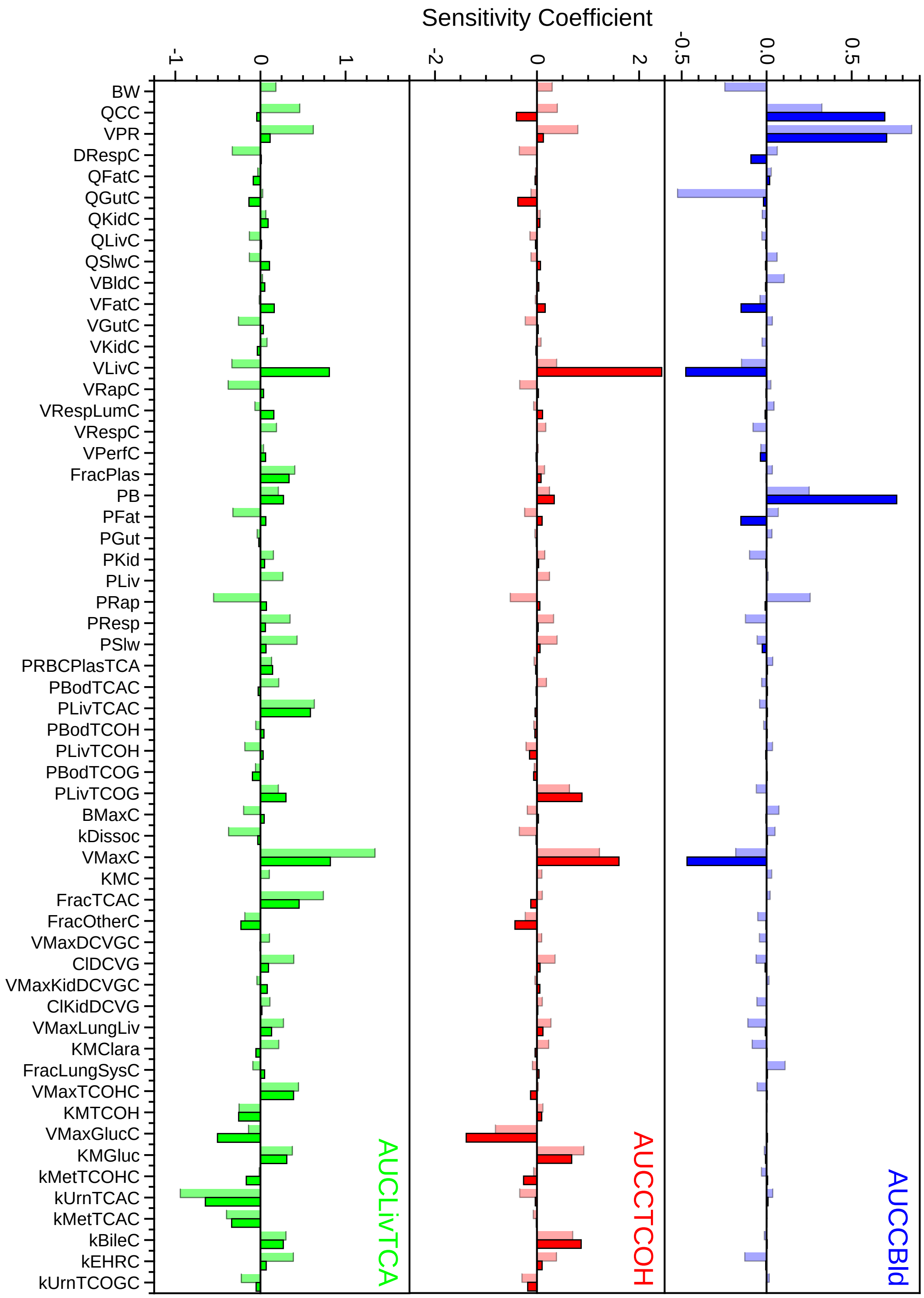

Figure 20. Sensitivity Coefficients for Rat Following Inhalation Exposure. Exposure was 100 (light bars) or 600 ppm (dark bars) for 7 hours/day, 5 days/week for 10 weeks. Sensitivity coefficients were calculated as fraction change in output per fraction change in input.

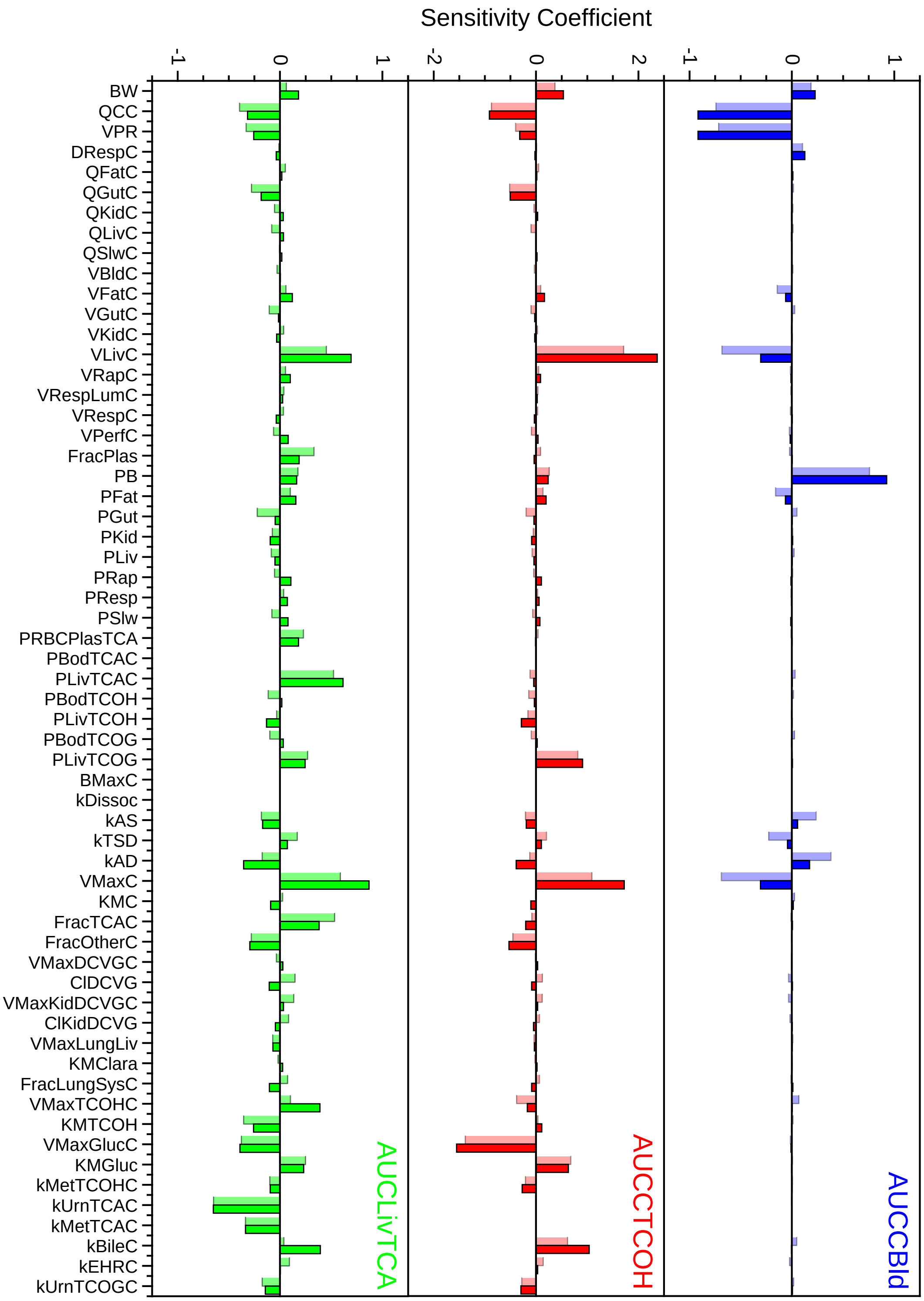

Figure 21. Sensitivity Coefficients for Rat Following Gavage Exposure. Exposure was 300 (light bars) or 1,000 mg/kg-day (dark bars) for 5 days/week for 10 weeks. Sensitivity coefficients were calculated using equation in EPA (2011).

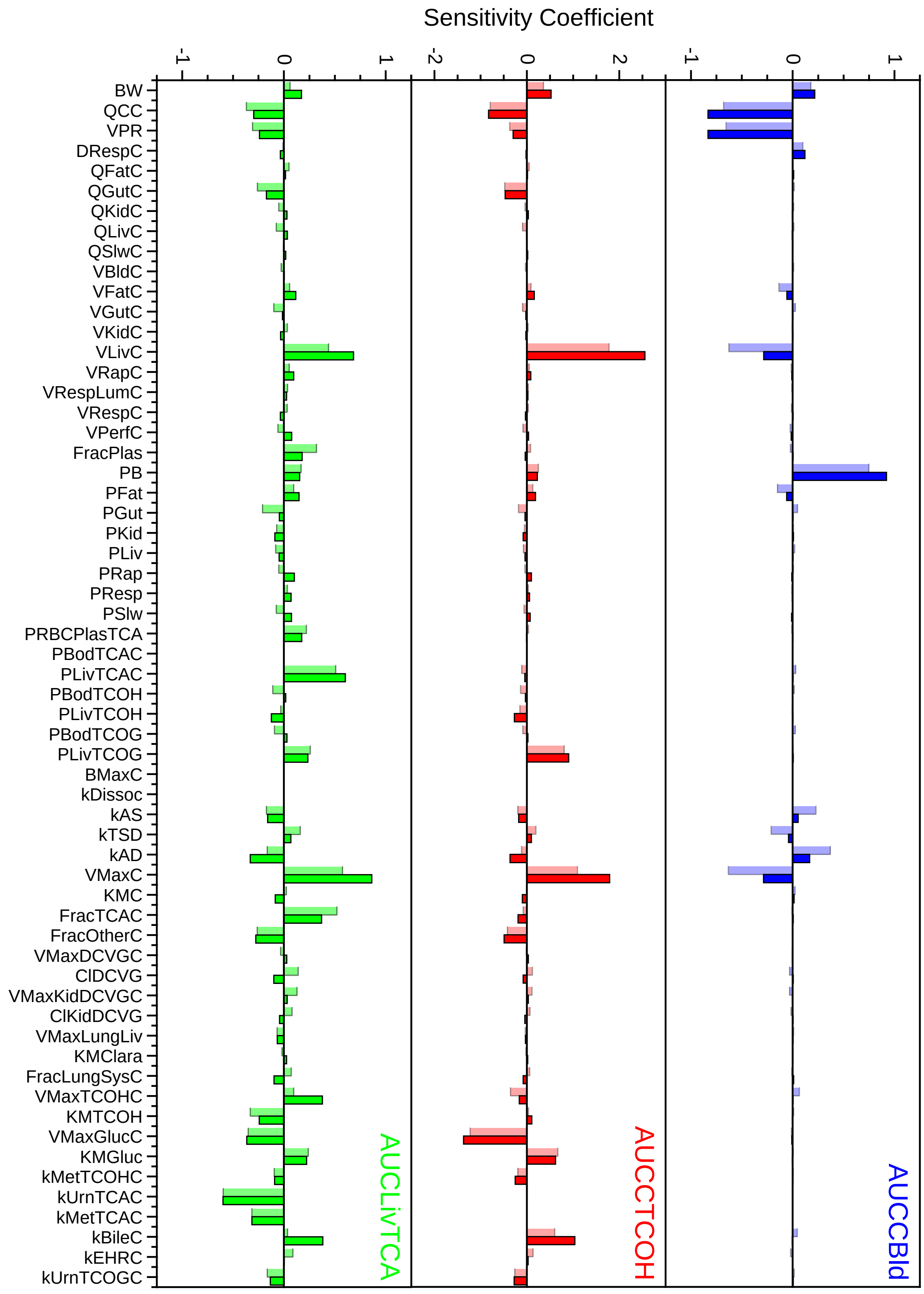

Figure 22. Sensitivity Coefficients for Rat Following Gavage Exposure. Exposure was 300 (light bars) or 1,000 mg/kg-day (dark bars) for 5 days/week for 10 weeks. Sensitivity coefficients were calculated as fraction change in output per fraction change in input.

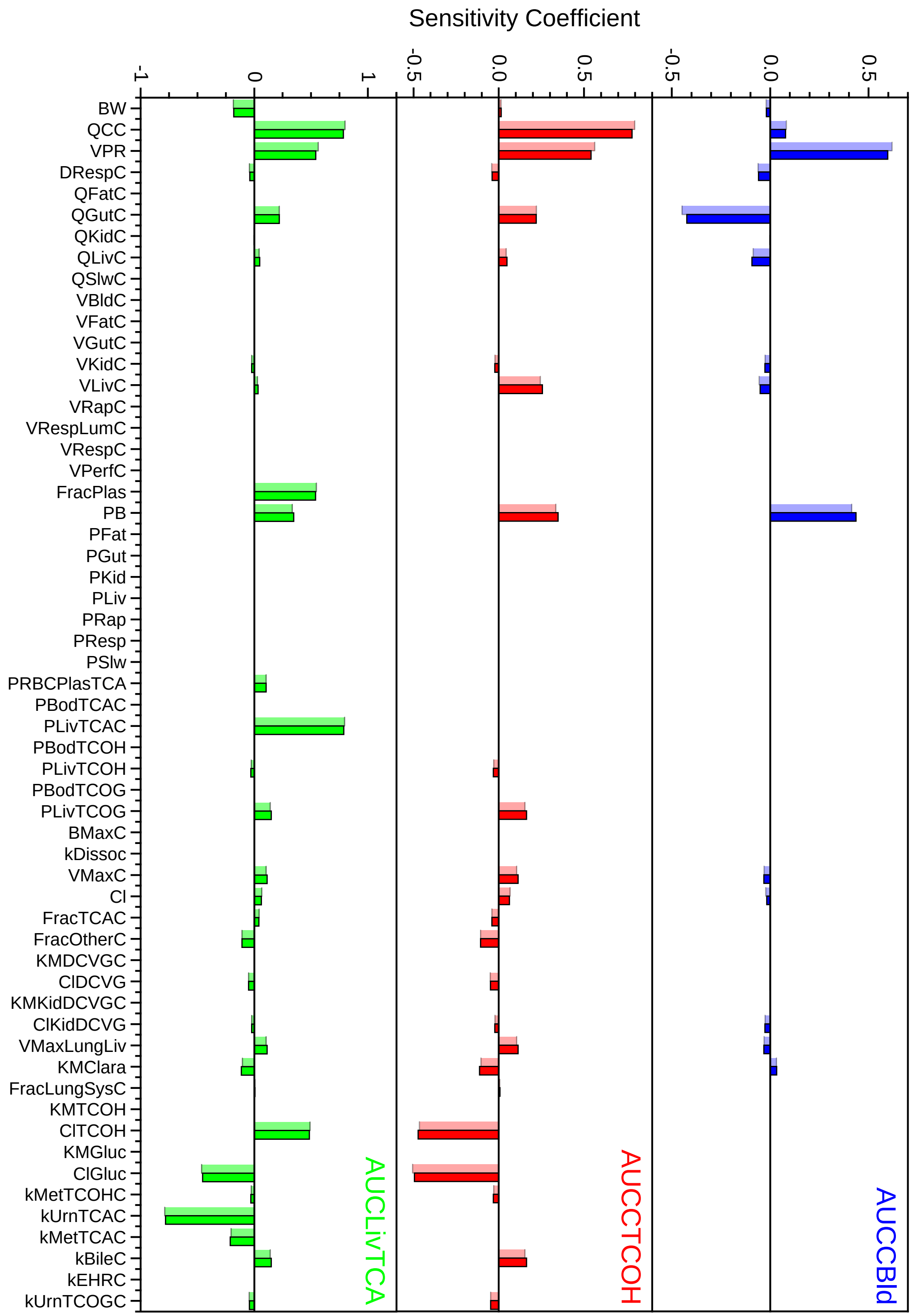

Figure 23. Sensitivity Coefficients for Human Following Inhalation Exposure. Exposure was continuous 0.001 ppm to females (light bars) or males (dark bars) for 100 weeks. Sensitivity coefficients were calculated using equation in EPA (2011).

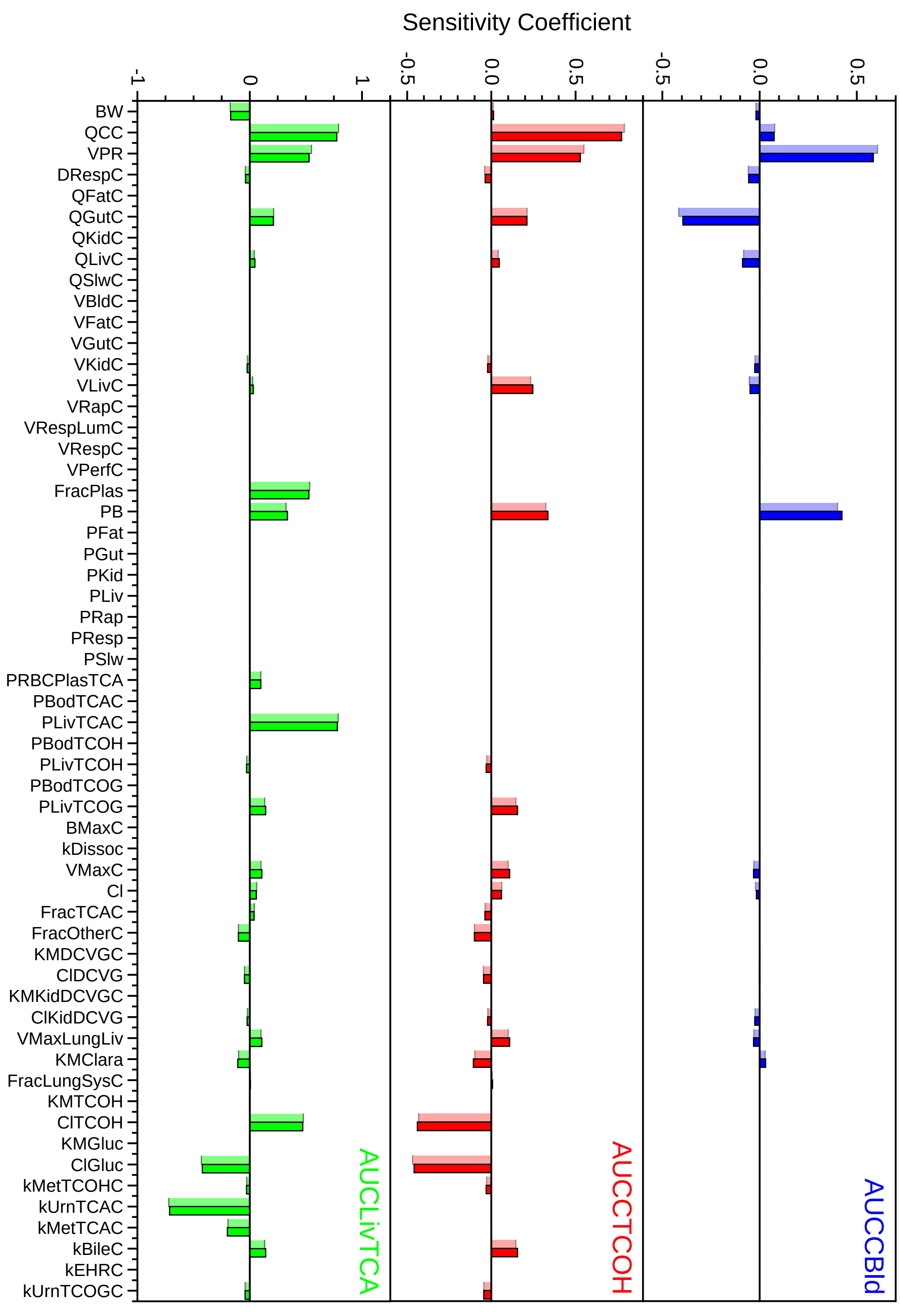

Figure 24. Sensitivity Coefficients for Human Following Inhalation Exposure. Exposure was continuous 0.001 ppm to females (light bars) or males (dark bars) for 100 weeks. Sensitivity coefficients were calculated as fraction change in output per fraction change in input.

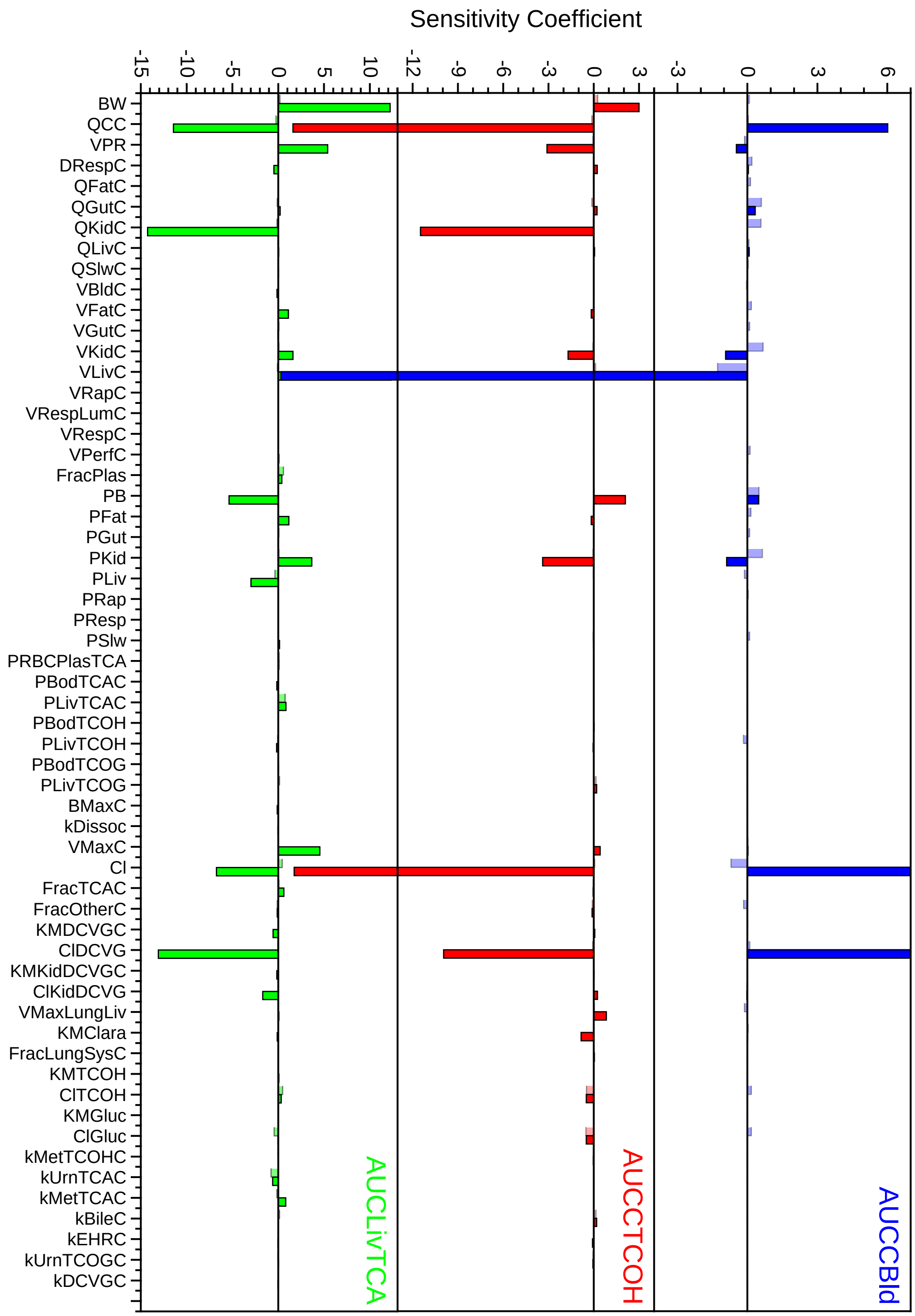

Figure 25a. Sensitivity Coefficients for Human Following Oral Exposure. Exposure was continuous 0.001 mg/kg-day to females (light bars) or males (dark bars) for 100 weeks. Sensitivity coefficients were calculated using equation in EPA (2011). Male values for bars that are cut off by axes are as follows: for AUCCBld – VLivC=-20.0, Cl=20.0, ClDCVG=20.0; for AUCCTCOH – QCC=-19.9, VLivC=19.8, Cl=-19.9.

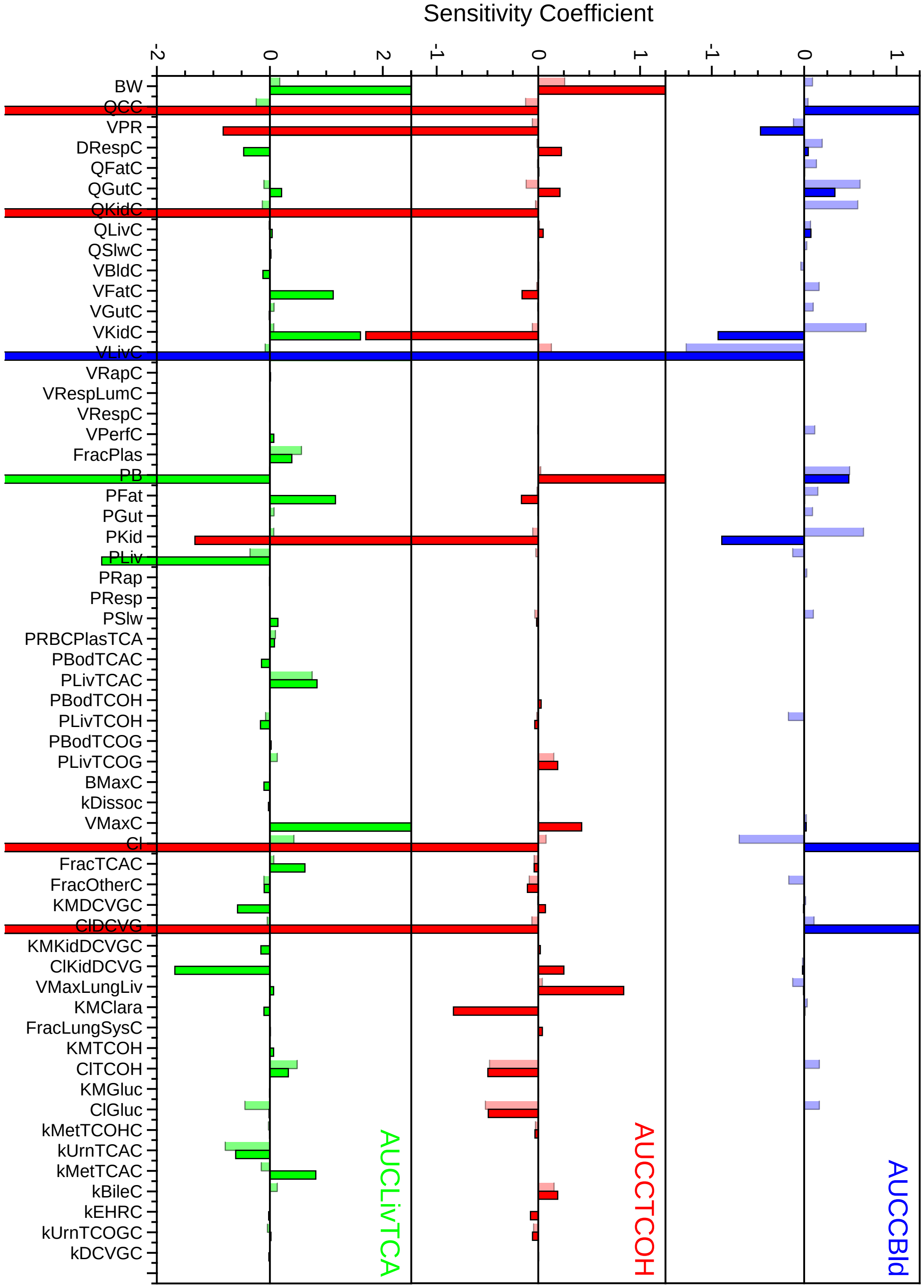

Figure 25b. Sensitivity Coefficients for Human Following Oral Exposure. Exposure was continuous 0.001 mg/kg-day to females (light bars) or males (dark bars) for 100 weeks. Sensitivity coefficients were calculated using equation in EPA (2011). Figure presents the same information as Figure 14a only with smaller axis limits so as to see the smaller values.

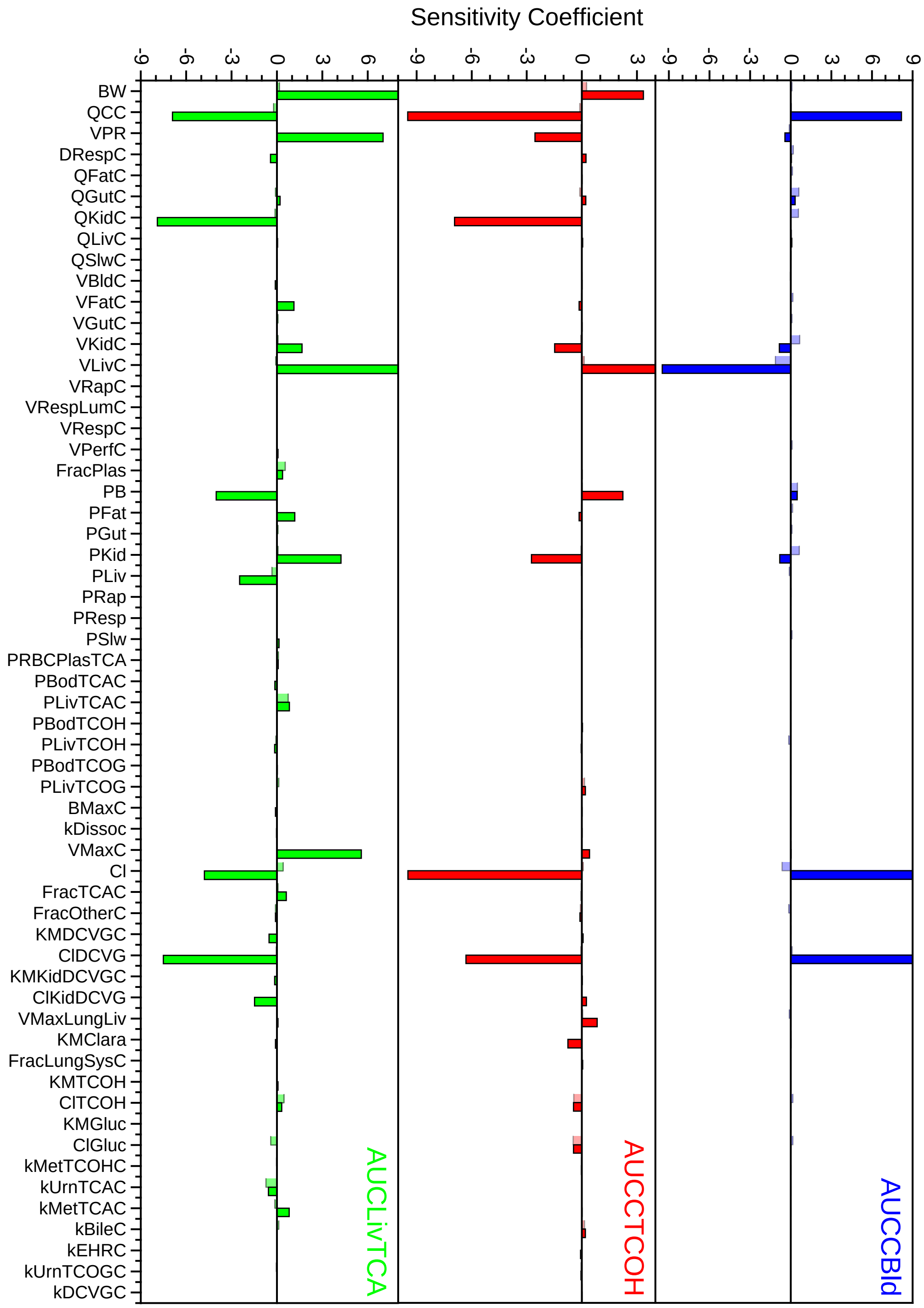

Figure 26a. Sensitivity Coefficients for Human Following Oral Exposure. Exposure was continuous 0.001 mg/kg-day to females (light bars) or males (dark bars) for 100 weeks. Sensitivity coefficients were calculated as fraction change in output per fraction change in input. Male values for bars that are cut off by axes are as follows: for AUCCBld –Cl=2.5e10, ClDCVG=1.9e10; for AUCCTCOH – VLivC=1618.0; for AUCLivTCA – BW=29.8, VLivC=30.4.

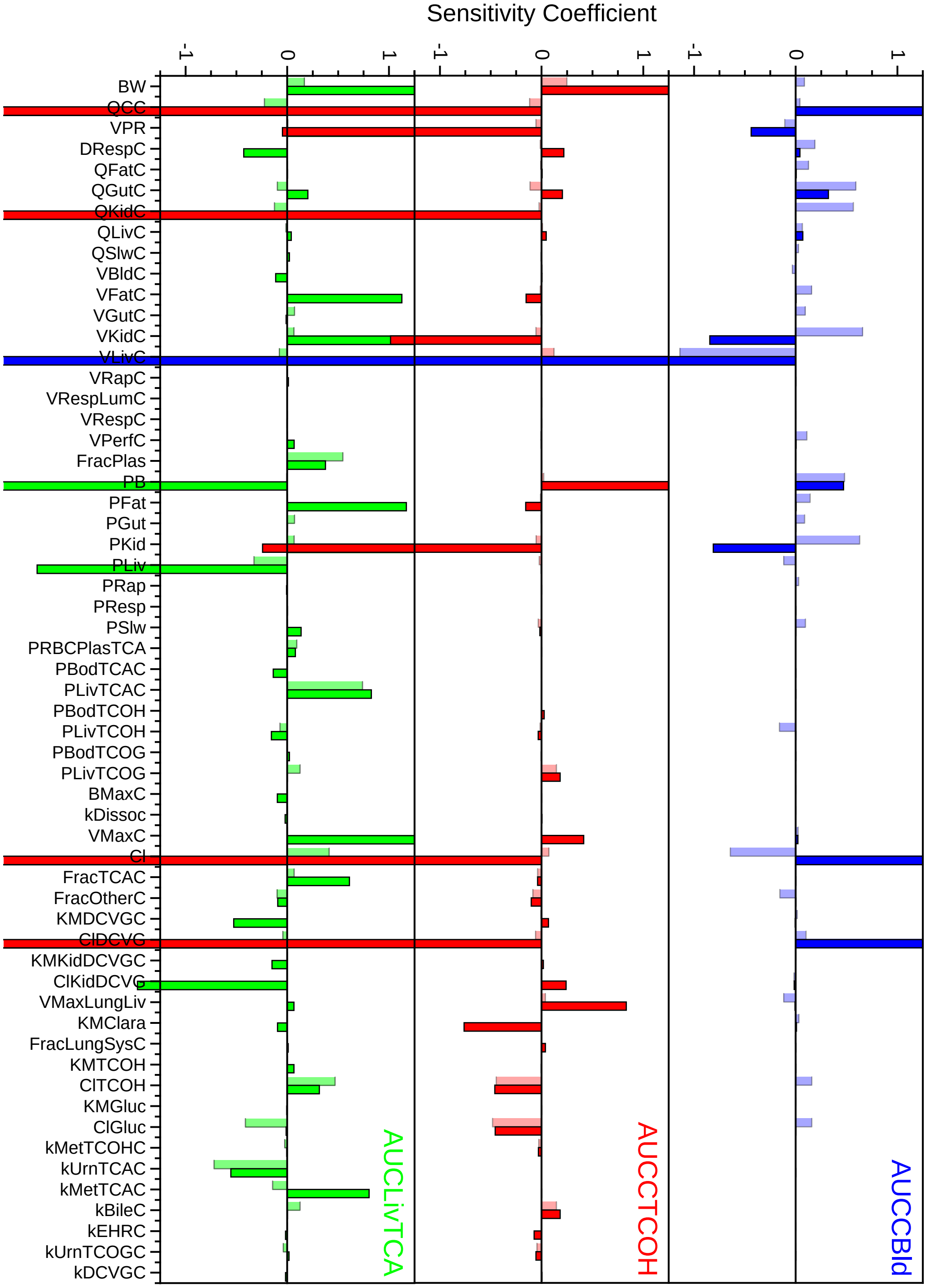

Figure 26b. Sensitivity Coefficients for Human Following Oral Exposure. Exposure was continuous 0.001 mg/kg-day to females (light bars) or males (dark bars) for 100 weeks. Sensitivity coefficients were calculated as fraction change in output per fraction change in input. Figure presents the same information as Figure 15a only with smaller axis limits so as to see the smaller values.

6.0 TASK 2B: EVALUATE EPA'S BAYESIAN METHOD FOR PRIOR VALIDATION AND THE IMPACT OF THEIR USE OF THE METHOD

6.1 Data Inclusion

EPA (2011) used both individual and grouped data. While individual data are preferred as it maintains any intra-individual variation, it is often not available, particularly in the case of animal data. It is not uncommon, therefore, for grouped data to be used for Markov Chain Monte Carlo (MCMC) analysis and for grouped data to be used along with individual data (David *et al.*, 2006; Marino *et al.*, 2006; Covington *et al.*, 2007). In using grouped data, the user would, ideally, account for the loss of intra-individual variation in some manner; however, there is not a commonly accepted method for this. Therefore, no problems are seen with how EPA (2011) handled the group data.

Specific endpoints included in the MCMC analysis by EPA (2011) were also evaluated. For DCVG blood concentration data, it is unclear as to exactly how the non-detect values were used or why they were included, as there are some data for this endpoint that are above the detection limit. The validity of using a value of half the detection limit is questionable, as the actual value is unknown. Even if half-detection values are only used for plotting purposes, one gains nothing by noting that the model over- or under-predicts these points, given that the plotted half-detection values may not reflect the actual very low (or essentially zero) concentrations. Use of these half-detection values would be especially problematic if the points were used for parameter estimation; it is unclear whether EPA (2011) used these data in this manner.

MCMC simulation in MCSim can be performed to analyze variability and uncertainty at population and individual or experimental levels. The hierarchy of levels designates how parameters are sampled for each run from initially defined parameter distributions, which are refined based on the observed data. For the animal studies, EPA (2011) included all of the data for a given study in the same level with separate experiments for dose. Therefore, all experiments for the given study, which were using the same animal strain, applied the same physiological and chemical specific parameters (with the possible exception of dose-group specific body weights).

This hierarchy is different than that used by Hack *et al.* (2006) who put each dose group in a separate level, thus allowing for each dose group, even within a study, to use different parameter values. EPA (2011) stated that they grouped the data for each study into a single level as they felt there would be little intra-animal variation within a given study. It should be noted that EPA (2011) did separate the Prout *et al.* (1985) rat data into two separate levels since this study used two different rat strains (Adderley Park and Osborne-Mendel). Either method is valid and precedented; no problems were found with how EPA (2011) defined their animal levels.

For the human data, separate exposure levels were again defined for each study, but additional levels were defined for each subject within the study with experiment levels for each dose. This allowed for different physiological and chemical specific parameters to be used for each individual. Hack *et al.* (2006) placed the data for each individual dose into a separate level thus

allowing for different parameters to be used for the same individual at the different dosing exposures. Given that the dosing exposures were not usually that far apart, changes in physiological or chemical specific parameters within an individual seems unlikely; therefore, the EPA (2011) hierarchy definition was an improvement over Hack *et al.* (2006).

6.2 Distribution Definitions

EPA (2011) states that they "redefined priors" by using a common underlying value for the parameter, defined distributions based on this scaling, and then updated the distributions with the MCMC analysis. They state that they use this scaling method to update the priors for the subsequent run based on the previous run (*i.e.*, to update rat priors based on mouse posteriors) and that the bounds on these updated priors are set wide enough such that if the "…data strongly imply an extreme species-specific value, they can be accommodated". The description of their scaling method is unclear and they state that it is "standard practice", but no references are given.

Typically what is seen are certain physiological and chemical specific parameters scaled by body weight (*e.g*., $QC=QCC*BW^{0.75}$) and then the distributions for the MCMC analysis are defined for the base parameter itself (*e.g*., QCC) rather than a fractional change in QCC as in EPA (2011). The method used by EPA (2011) seems to add a great deal of complexity and it's not clear that anything is really gained in the end. If the bounds on the distribution are set wide enough to allow extreme species-specific values, then using, for instance, the mouse posteriors as the rat priors in addition to the wide bounds should be sufficient to allow the MCMC analysis to reach the same posterior results if sufficient iterations and chains are used. Given that they also presented their posterior results as either the fractional changes or parameter changes for parameters that are not directly input into the model (*e.g.*, giving a posterior value for QPC when the model requires VPR and calculates QPC), it requires more effort to determine the actual posterior values that should be used to run in the model.

EPA (2011) also mentioned concerns over using "fit" values for the prior mean and thereby biasing the results. Again, if the analysis is run for a sufficient length of time with a sufficient number of chains and the distributions are defined broad enough, the analysis should still be able to update the posterior distributions without being constrained by using a "fit" value as the prior mean.

It was also noted that EPA (2011) updated the distributions for physiological parameters that are typically considered to be well defined from the literature (*i.e*., tissue blood flows and volumes). While this is not a problem with the analysis, it could add to the amount of time required to complete the desired number of iterations; EPA (2011) did state that certain chains were shorter than others due to computational constraints.

The parameter distributions for the means were typically defined using either normal or log-normal distributions. For the log-normal distributions, log-transformed versions of the parameters were calculated and then distributions were defined for these log-transformed parameters with a normal distribution. However, a few of the parameters (more associated with mouse and rat than for human) were defined using log-uniform distributions (uniform

distributions on log-transformed parameters). These parameters are those that are probably the least likely to have been measured and are often fit to the data. No references or justifications were given for this decision. It can be hypothesized that uniform and log-uniform distributions were used because little is known on what the true distribution would be for these parameters; thus, EPA (2011) assumed that any given value would be equally likely to be any other value between the defined bounds. This approach is atypical. Assuming that any value between the defined bounds is equally likely as any other seems less plausible than assuming a normal or log-normal distribution with sufficiently wide bounds. It's not clear how the definition of these distributions would affect the results of EPA (2011), but at the very least, it seems it might cause the analysis to take longer to converge. The parameters for which uniform or log-uniform distributions were used are listed below in alphabetical order.

- For mouse: ClDCVGC, ClKidDCVGC, DRespC, FracKidDCVCC, FracLungSysC, FracOtherC, kAD, kAS, kASTCA, kASTCOH, kBileC, kDCVGC, kEHRC, kKidBioactC, KMClara, kMetTCAC, kMetTCOHC, KMGluc, KMTCOH, kNATC, kTD, kTSD, kUrnTCAC, kUrnTCOGC, PBodTCOGC, PEffDCVG, PLivTCOGC, PRBCPlasTCAC, VMaxDCVGC, VMaxGlucC, VMaxKidDCVGC, VMaxTCOHC
- For rat: ClDCVGC, ClKidDCVGC, FracLungSysC, FracOtherC, FracTCAC, kAD, kAS, kASTCA, kASTCOH, kBileC, kEHRC, kKidBioactC, KMC, KMClara, kMetTCAC, kMetTCOHC, KMGluc, KMTCOH, kNATC, kTD, kTSD, kUrnTCAC, kUrnTCOGC, VMaxC, VMaxDCVGC, VMaxGlucC, VMaxKidDCVGC, VMaxLungLivC, VMaxTCOHC
- For human: kASTCA, kASTCOH, kDCVGC, PRBCPlasTCAC, PEffDCVG

EPA (2011) also stated that they used the same prior definitions for residual errors for all mouse studies, but for rat and human they used different definitions for different studies. In looking at the MCSim files provided in the supplemental data, the definitions look to all be the same. It's unclear why there is discrepancy between the text and MCSim files. EPA (2011) justified the use of different definitions for the prior residual errors by stating that using the same definitions led to large posterior residual errors even though the fits were reasonable. However, using different definitions seems random and, without documented precedence, questionable. It should be noted that the large posterior residual errors were potentially the result of errors in the model rather than errors in the prior definitions.

6.3 Execution of MCMC Analysis

EPA (2011) states that they ran the MCMC analysis sequentially for the three species data (*i.e.*, mouse first, followed by rat, and then by human) and that they ran four chains for each species. The number of iterations they ran varied by species due to computational constraints and the number of iterations required to have the chains converge. This is not uncommon. They ran one more chain than Hack *et al.* (2006) and ran the chains for more iterations; this is a potential improvement over the Hack *et al.* (2006) analysis. EPA (2011) also states that they restarted some of the chains to get additional iterations but they gave no details on how this was accomplished. The authors also stated, that due to computational constraints, the chains for a given species were not all run for the same number of iterations. The number of iterations per

chain looked to differ by 10,000 to 20,000 iterations. There doesn't seem to be any benefit from having some chains being so much longer than others, as any chain lengths beyond the length of the shortest chain should be discarded for final analysis. Computational time might perhaps have been better used running one less chain and running all chains for the same number of iterations, therefore weighing data from the analysis equally.

For the most part, the resulting posterior parameter estimates seem to meet a commonly employed criteria for convergence (R value less than or equal to 1.1; Sinharay, 2003). There were a few parameters for the rat and human for which the R values were above 1.1. The highest for the rat was the fraction of hepatic TCE oxidation not forming TCA and TCOH (FracOther, R of 1.44) and for the human was the elimination rate of TCOG in bile (kBileC, R=1.46). Some human parameters for which the R values were larger than 1.1 were important parameters for simulating inhalation exposure (*e.g.*, respiratory tract diffusion constant, DRespC).

7.0 TASK 3: DEVELOP DELIVERABLES DESCRIBING METHODS USED AND OUTCOMES OF TASKS

This report fulfills the requirements for Task 3.

8.0 CONCLUSIONS

There clearly appear to be some issues with the EPA (2011) model code that need to be addressed prior to using the model. The code, as is, predicts negative values for parameters and exhibits instability for some of the runs. While some of the validation figures appear to match those in EPA (2011), others do not; some figures are markedly different. Given that the shape of the predicted simulations were similar to those in EPA (2011), it is felt that the discrepancies could be due to the use of different posterior parameters due to the difficulty in determining which posterior values were in EPA (2011). The discrepancies may also be a difference between using subject-specific posteriors parameter values, as EPA (2011) states were used, and using population posterior parameter values which were applied here as the subject-specific parameters were not provided in EPA (2011).

The results for the sensitivity analysis seem to be similar to those of EPA (2011) with the exception of some outlying values. Most of the coefficients also seem to be fairly reasonable with the exception of these outlying values. Given the instability of the model and the parameters for which these outlying values were calculated, it seems likely that these values are more a result of model instability rather than model sensitivity. Conducting the sensitivity analysis proved quite useful in the discovery that the model instability was most noticeable in this process.

In general, the only major issue with how EPA (2011) conducted their Bayesian analysis was their use of uniform and log-uniform distributions for some of the parameters with no justification or references given for using these distributions. With sufficient iterations and chains, the analysis should still converge to mean values that would be obtained using different

distributions; however, it leaves open for discussion how useful it is to have uniform or log-uniform posterior distributions for these parameters.

There were some minor issues with their analysis. For instance, there was some uncertainty as to how they defined their priors and if their methods produced different results than methods used by other analyses (Covington *et al.*, 2007; Marino *et al.*, 2006). It also seems that it would have been more consistent if their chains for a given species were the same lengths. Another minor issue is their use of half of the non-detect value in the analysis. Overall, the issues with how EPA (2011) conducted their Bayesian analysis seem to be overshadowed by the issues in the model itself.

9.0 REFERENCES

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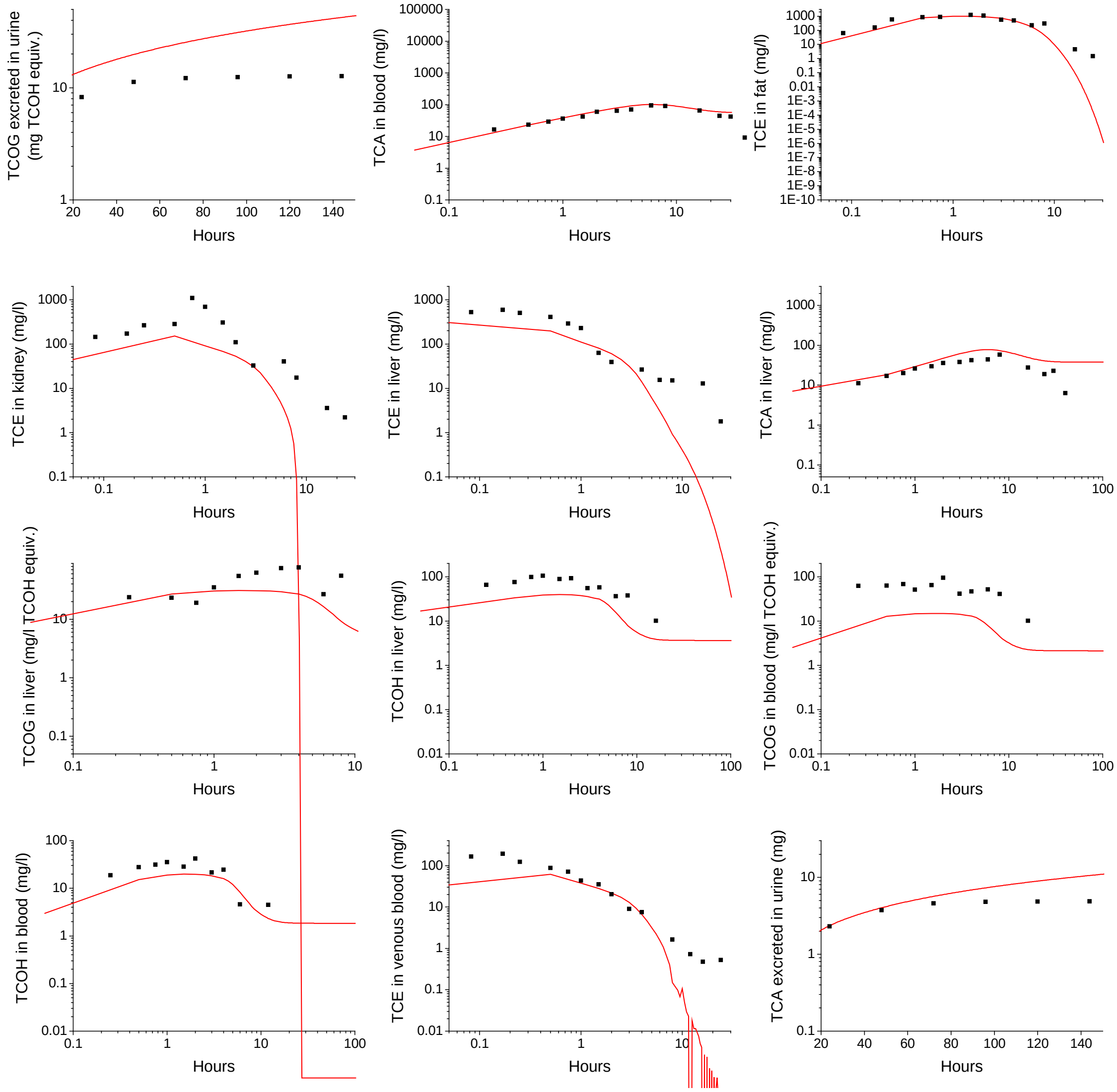
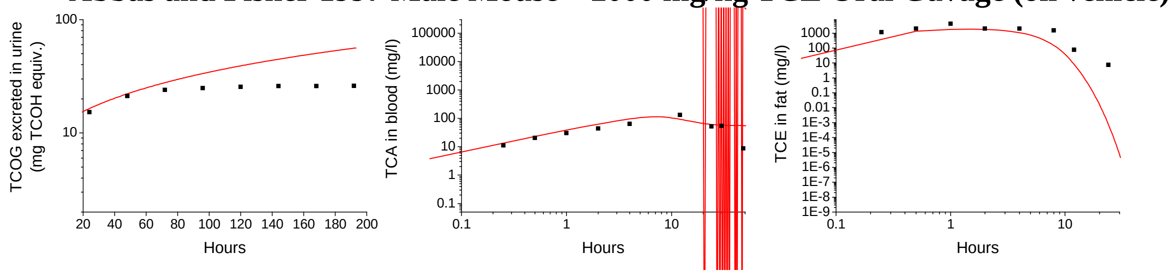
APPENDIX A. MOUSE VALIDATION FIGURES

Mouse figures correspond to Figure A-31 in EPA (2011). Red lines represent acslX model simulations using posterior population means. Citations for the original studies for these data are in the Section 9.0 of the main report.

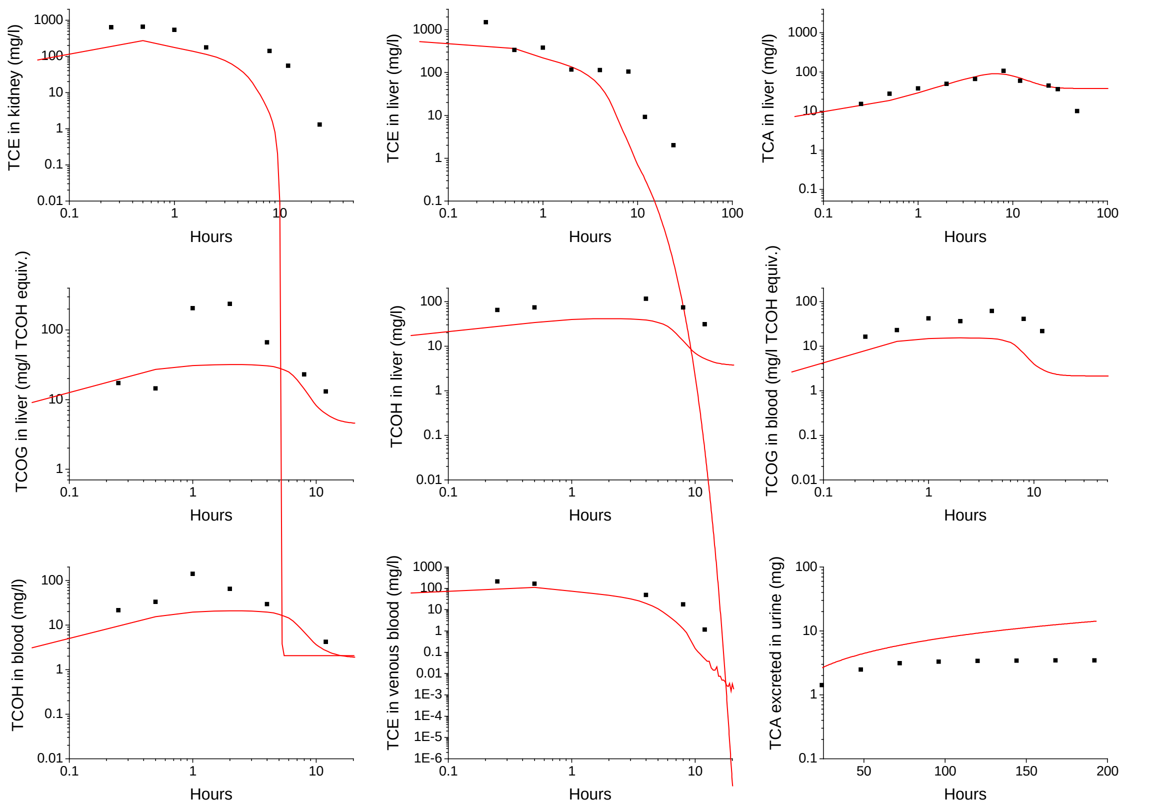
Abbas and Fisher 1997 Male Mouse – 1200 mg/kg TCE Oral Gavage (oil vehicle)



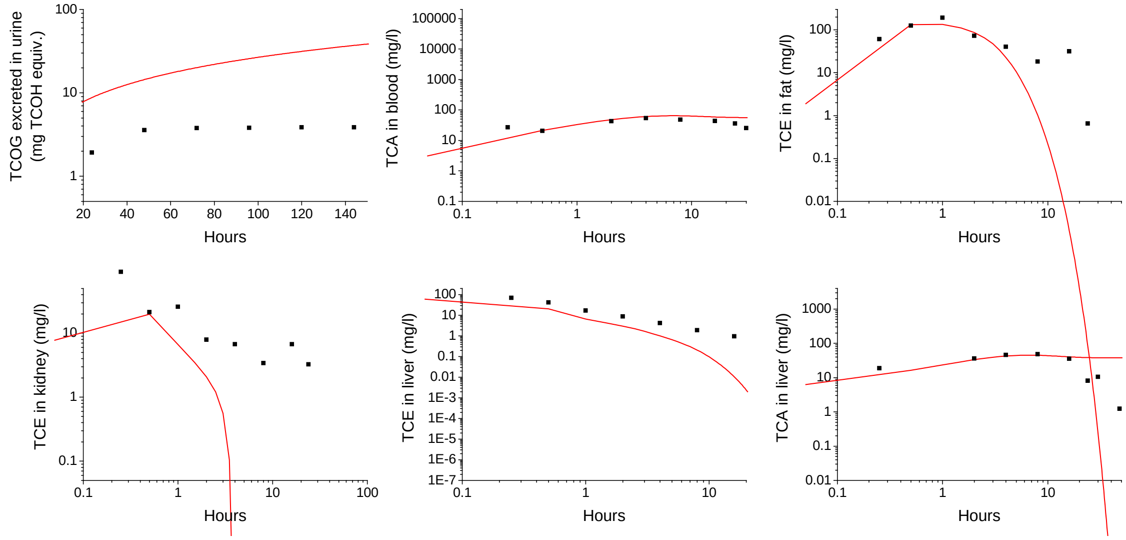
Abbas and Fisher 1997 Male Mouse – 2000 mg/kg TCE Oral Gavage (oil vehicle)



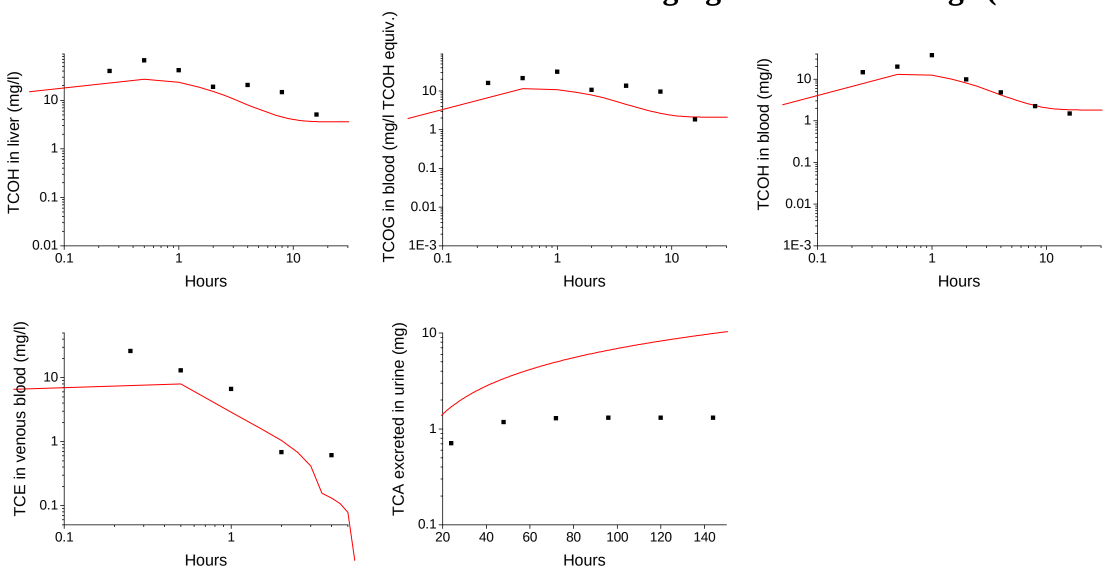
Abbas and Fisher 1997 Male Mouse – 2000 mg/kg TCE Oral Gavage (oil vehicle)



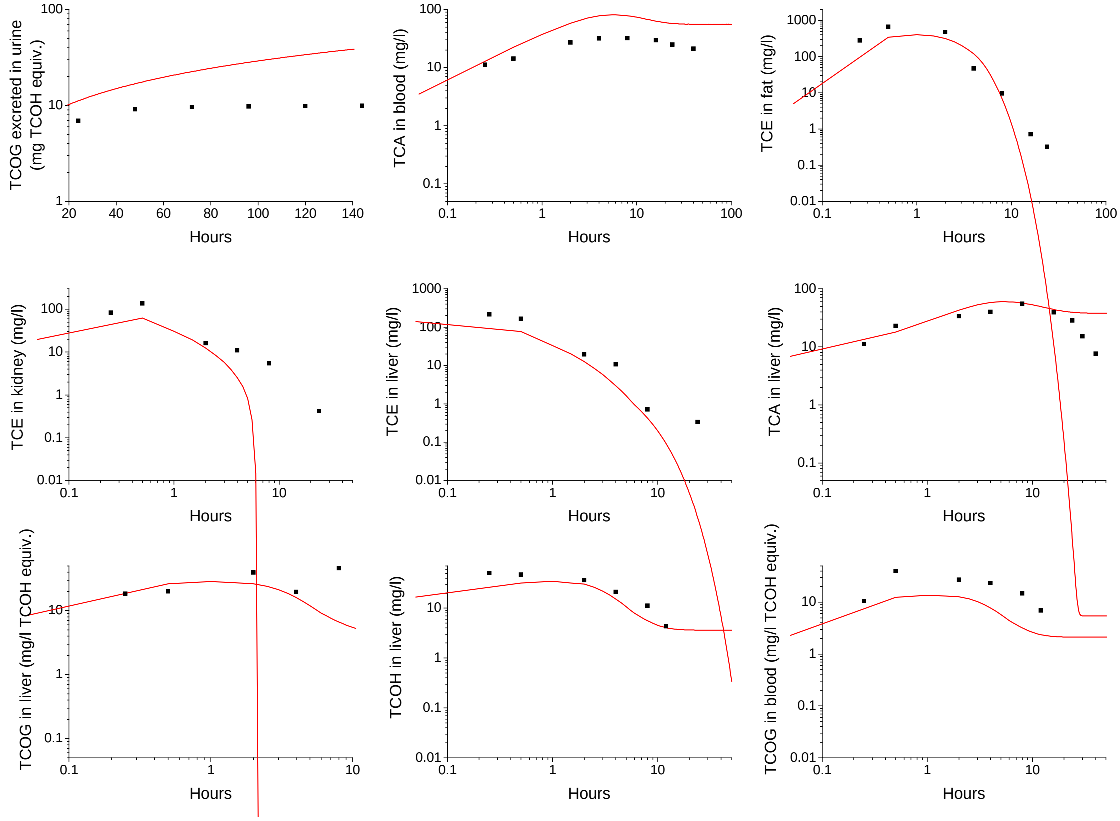
Abbas and Fisher 1997 Male Mouse – 300 mg/kg TCE Oral Gavage (oil vehicle)



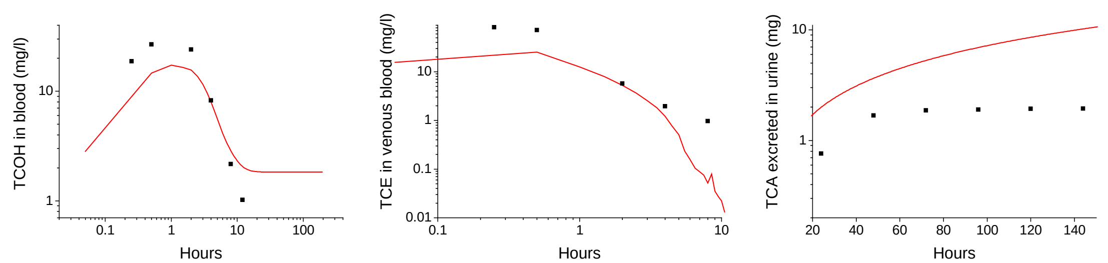
Abbas and Fisher 1997 Male Mouse – 300 mg/kg TCE Oral Gavage (oil vehicle)



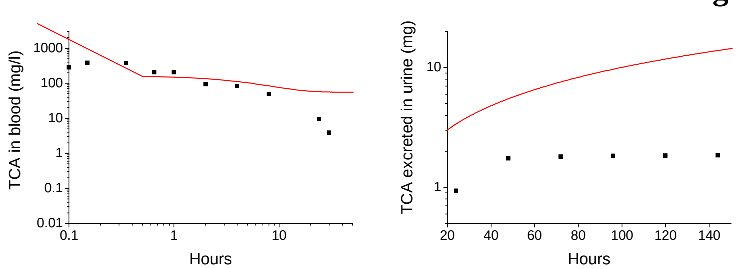
Abbas and Fisher 1997 Male Mouse – 600 mg/kg TCE Oral Gavage (oil vehicle)



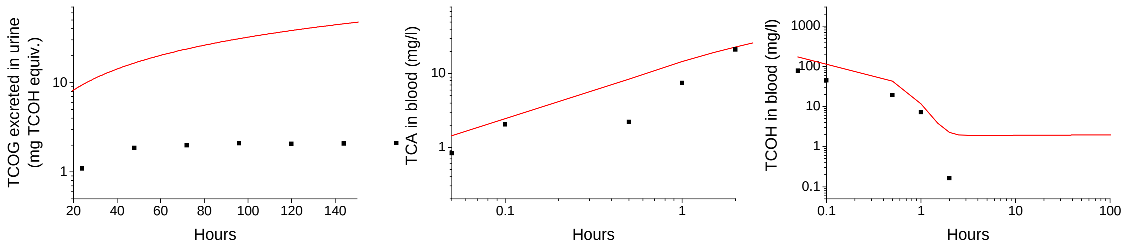
Abbas and Fisher 1997 Male Mouse – 600 mg/kg TCE Oral Gavage (oil vehicle)



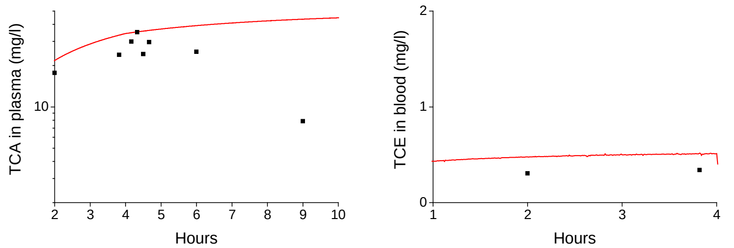
Abbas *et al.* 1997 Male Mouse – 100 mg/kg TCA Intravenous



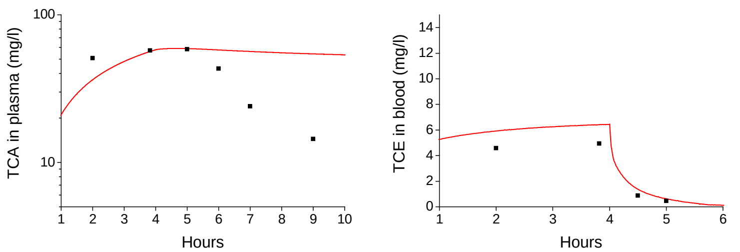
Abbas *et al.* 1997b Male Mouse – 100 mg/kg TCOH Intravenous



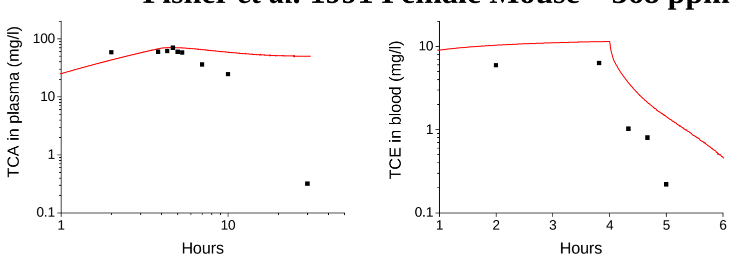
Fisher *et al.* 1991 Female Mouse – 42 ppm TCE 4 hour Inhalation



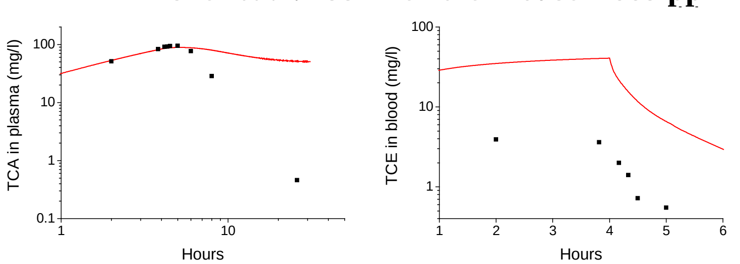
Fisher *et al.* 1991 Female Mouse – 236 ppm TCE 4 hour Inhalation



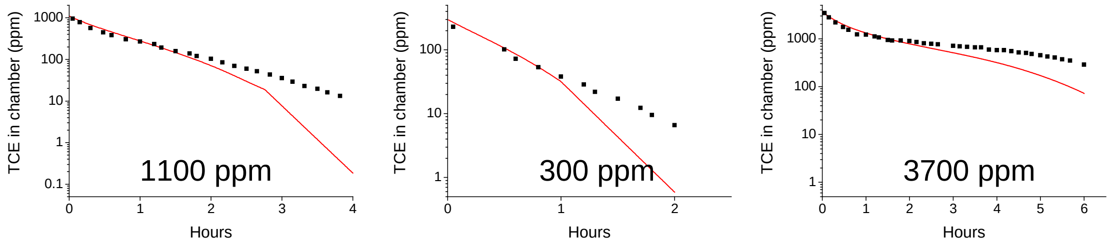
Fisher *et al.* 1991 Female Mouse – 368 ppm TCE 4 hour Inhalation



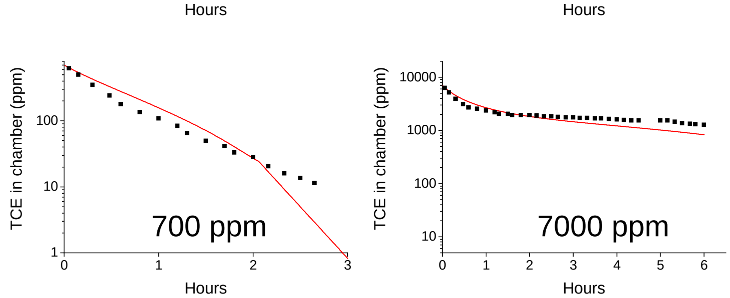
Fisher *et al.* 1991 Female Mouse – 889 ppm TCE 4 hour Inhalation



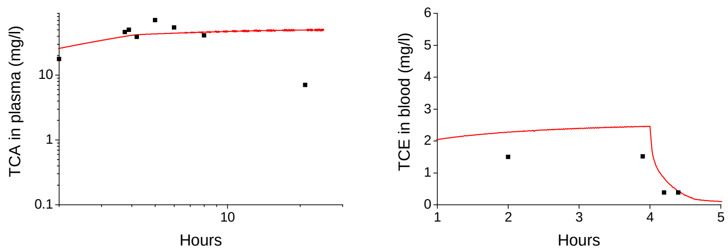
Fisher *et al.* 1991 Female Mouse – TCE Closed Chamber



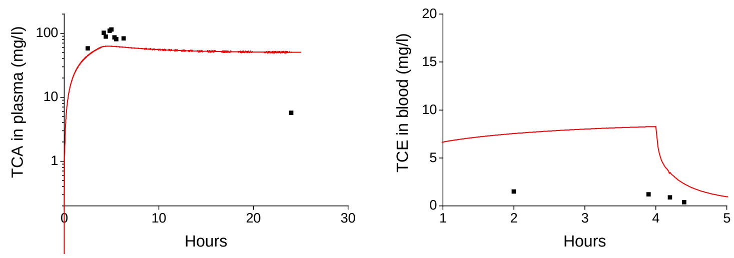
Fisher *et al.* 1991 Female Mouse – TCE Closed Chamber



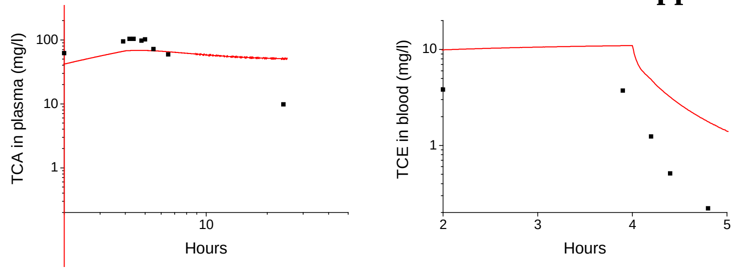
Fisher *et al.* 1991 Male Mouse – 110 ppm TCE 4 hour Inhalation



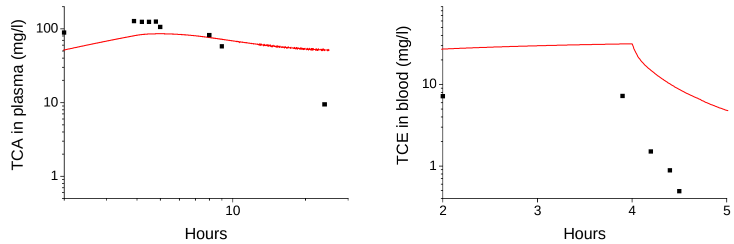
Fisher *et al.* 1991 Male Mouse – 297 ppm TCE 4 hour Inhalation



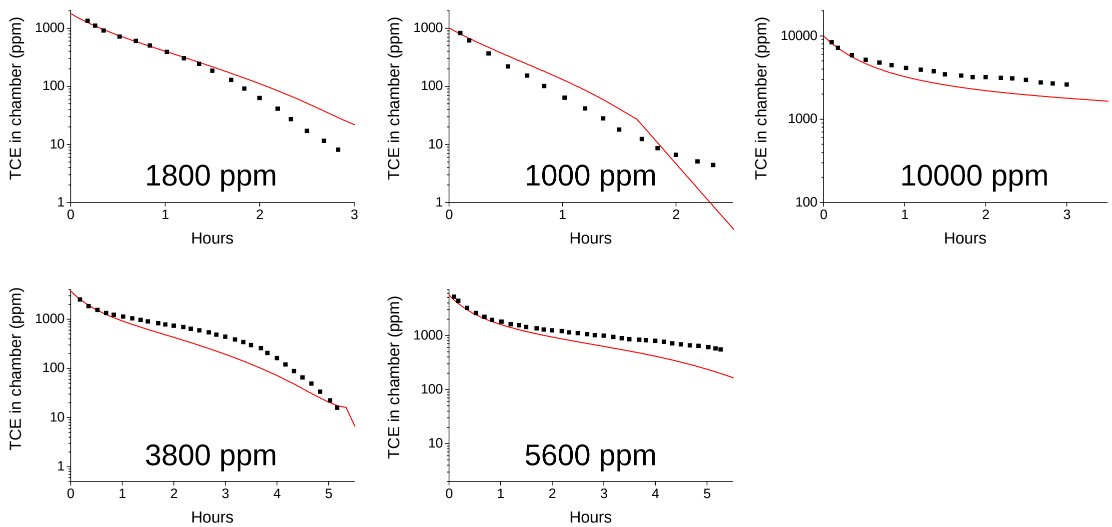
Fisher *et al.* 1991 Male Mouse – 368 ppm TCE 4 hour Inhalation



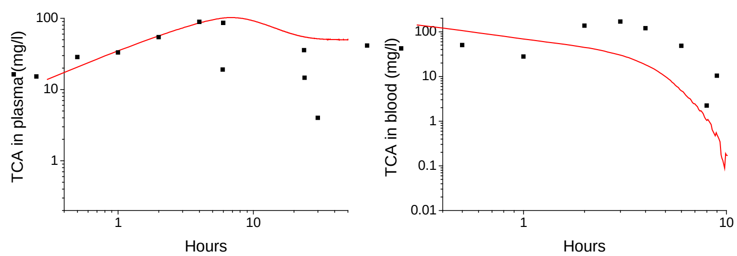
Fisher *et al.* 1991 Male Mouse – 748 ppm TCE 4 hour Inhalation



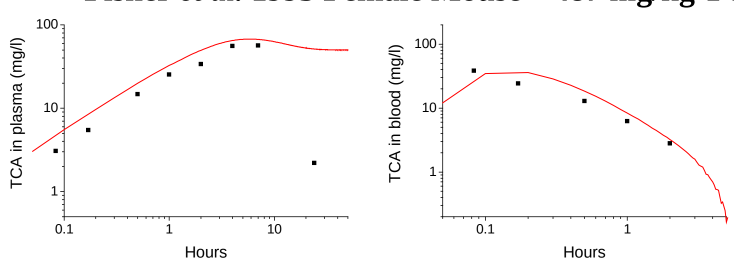
Fisher *et al.* 1991 Male Mouse – TCE Closed Chamber



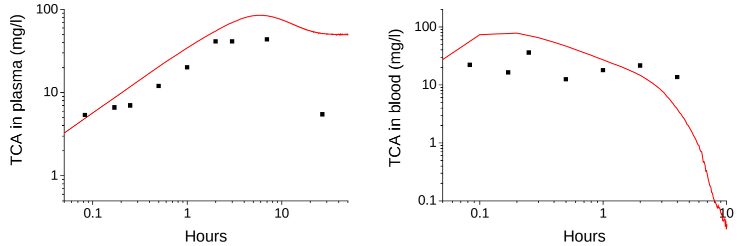
Fisher *et al.* 1993 Female Mouse – 2000 mg/kg TCE Oral Gavage (oil vehicle)



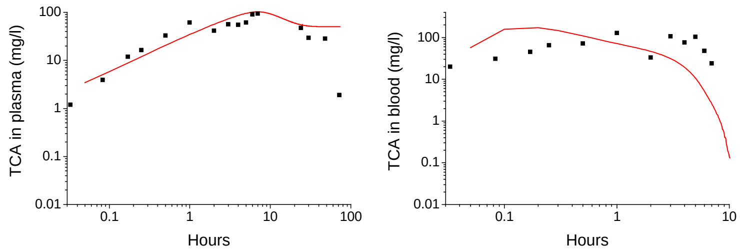
Fisher *et al.* 1993 Female Mouse – 487 mg/kg TCE Oral Gavage (oil vehicle)



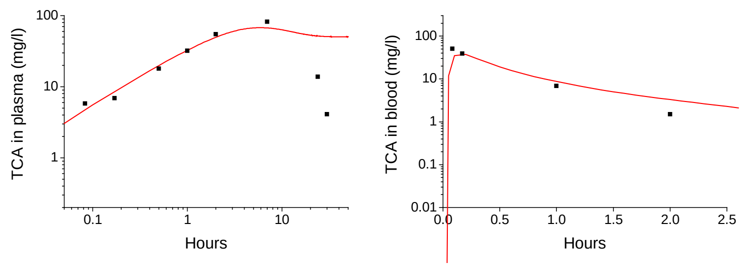
Fisher *et al.* 1993 Female Mouse – 973 mg/kg TCE Oral Gavage (oil vehicle)



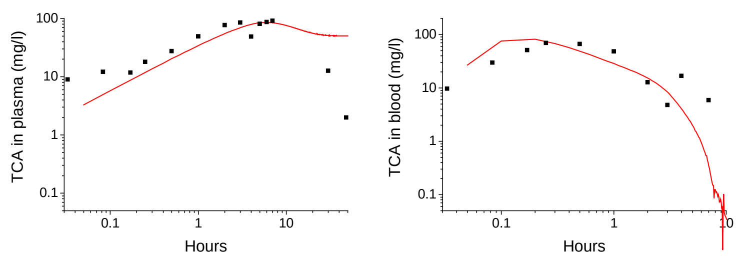
Fisher *et al.* 1993 Male Mouse – 2000 mg/kg TCE Oral Gavage (oil vehicle)



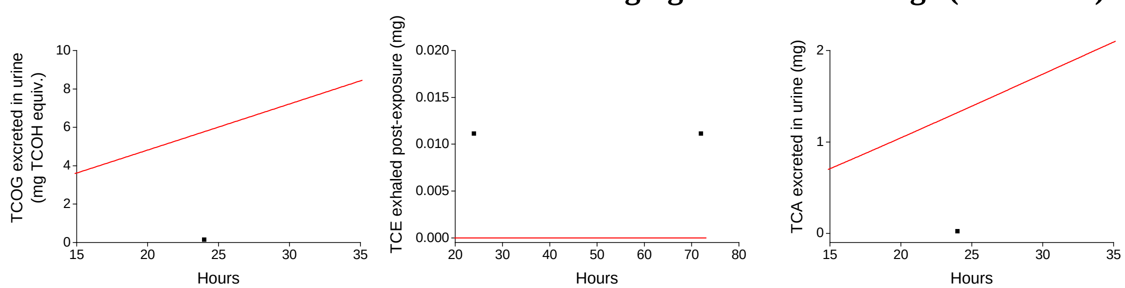
Fisher *et al.* 1993 Male Mouse – 487 mg/kg TCE Oral Gavage (oil vehicle)



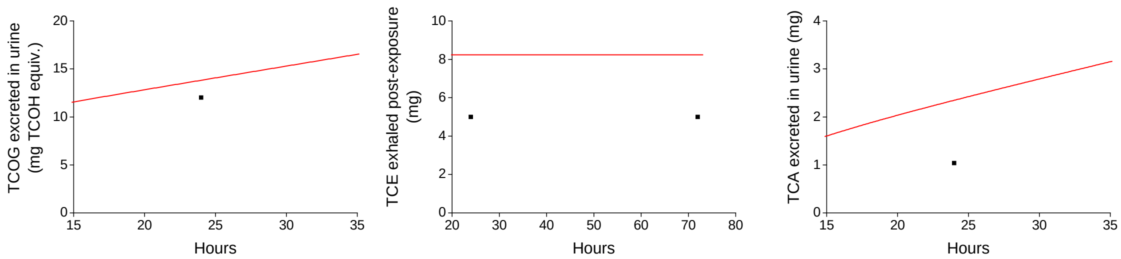
Fisher *et al.* 1993 Male Mouse – 973 mg/kg TCE Oral Gavage (oil vehicle)



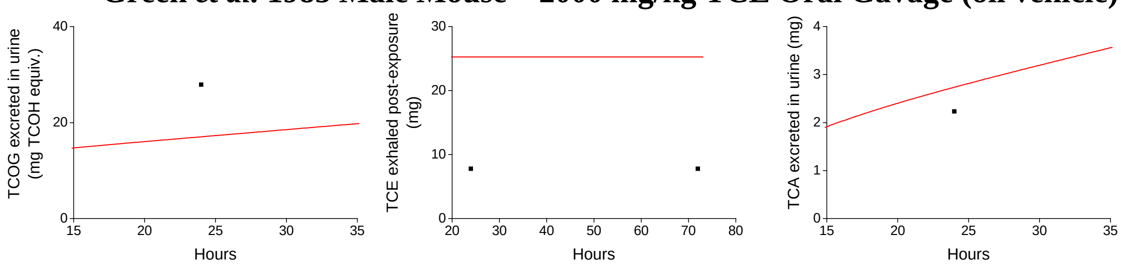
Green *et al.* 1985 Male Mouse – 10 mg/kg TCE Oral Gavage (oil vehicle)



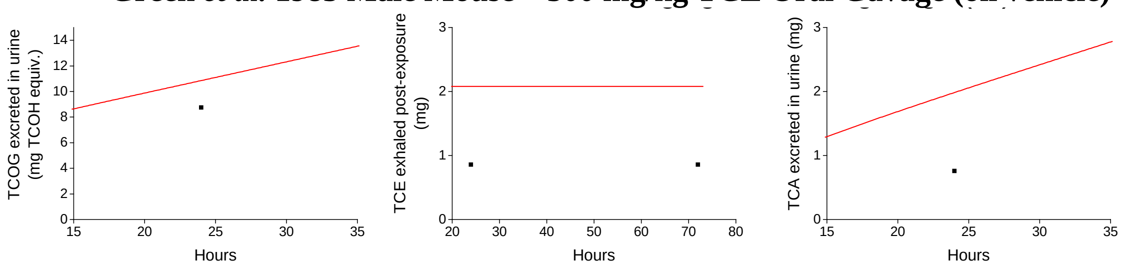
Green *et al.* 1985 Male Mouse – 1000 mg/kg TCE Oral Gavage (oil vehicle)



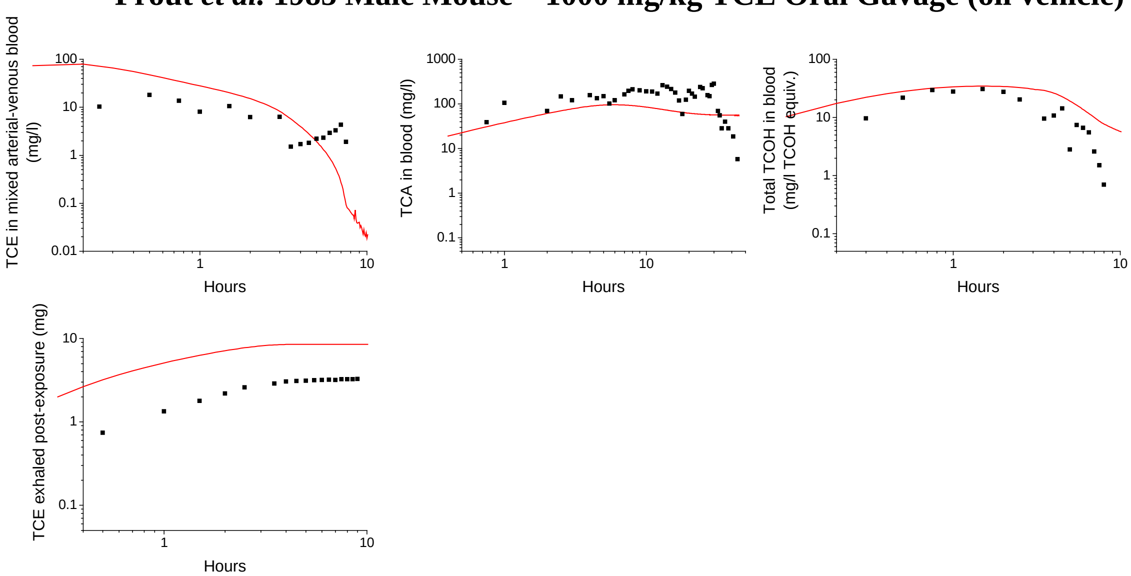
Green *et al.* 1985 Male Mouse – 2000 mg/kg TCE Oral Gavage (oil vehicle)



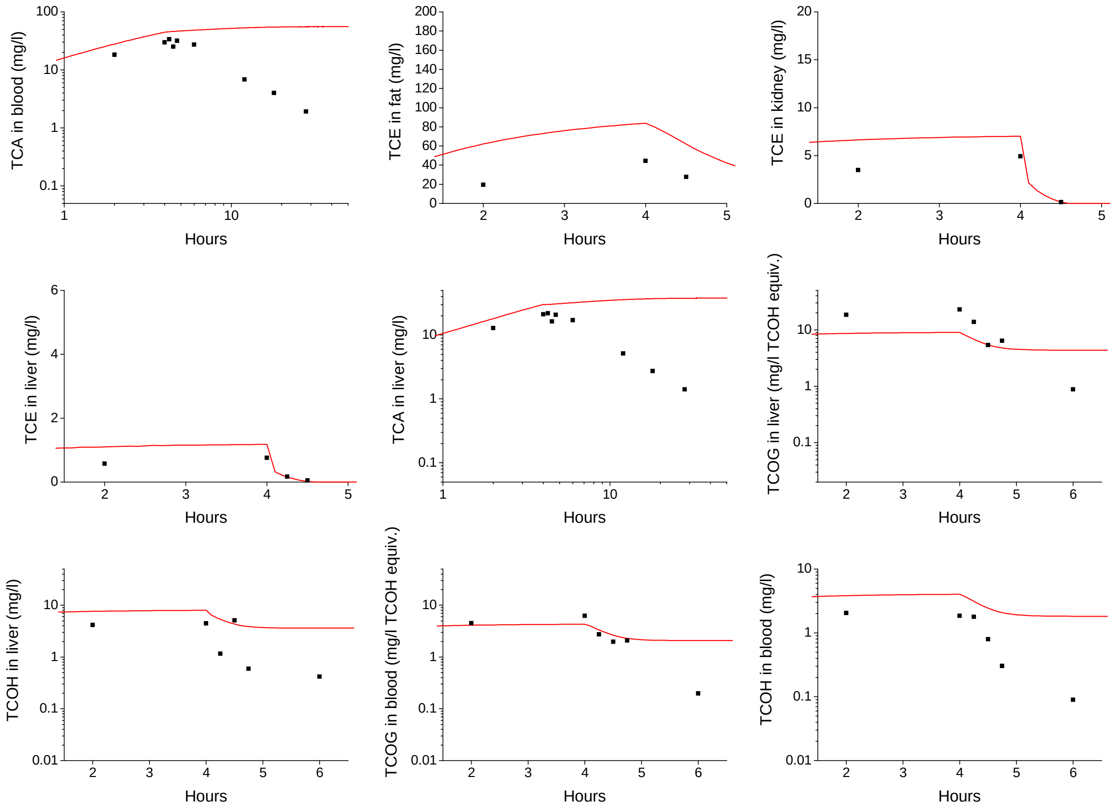
Green *et al.* 1985 Male Mouse – 500 mg/kg TCE Oral Gavage (oil vehicle)



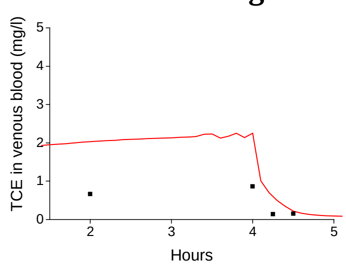
Prout *et al.* 1985 Male Mouse – 1000 mg/kg TCE Oral Gavage (oil vehicle)



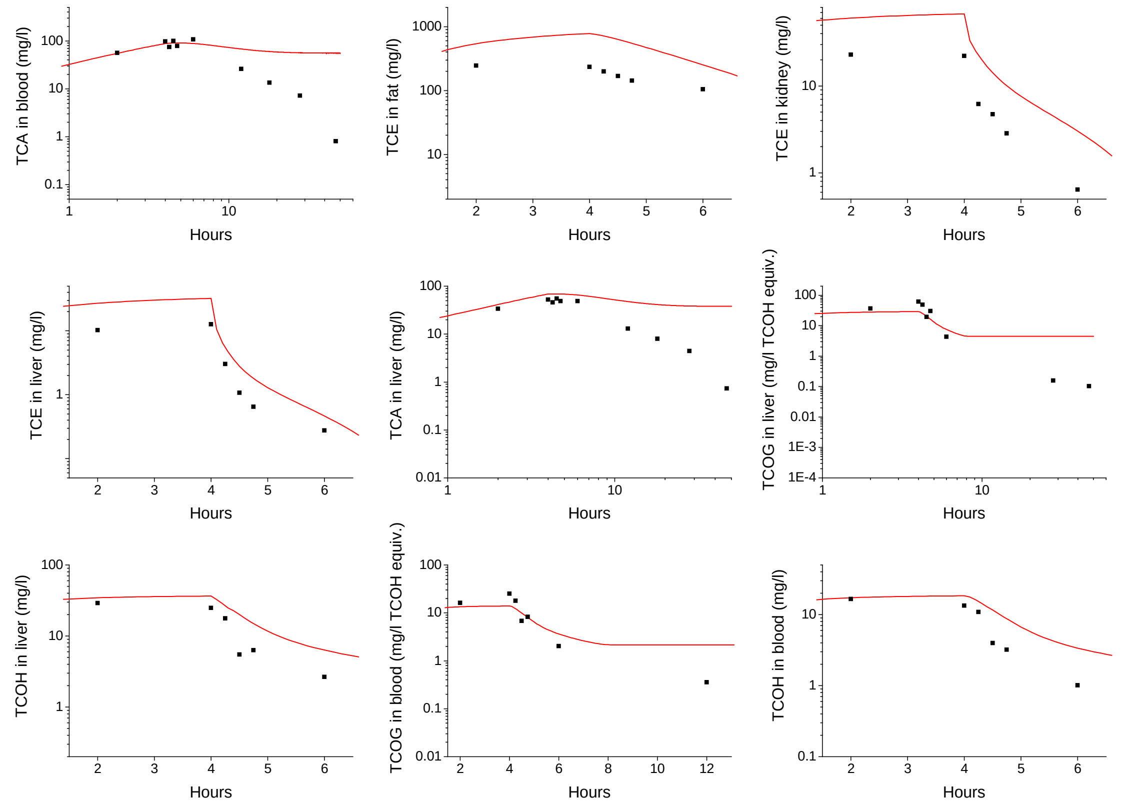
Greenberg *et al.* 1999 Male Mouse – 100 ppm TCE 4 hour Inhalation



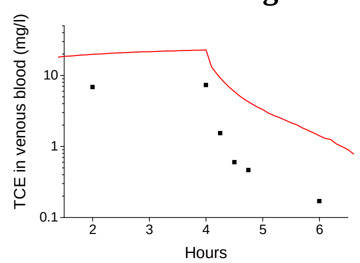
Greenberg *et al.* 1999 Male Mouse – 100 ppm TCE 4 hour Inhalation



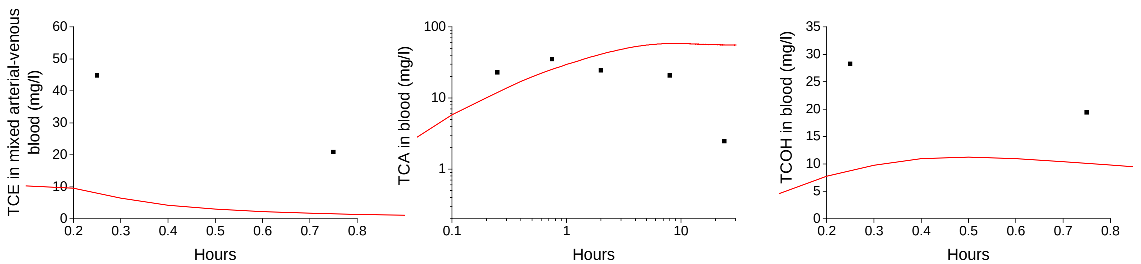
Greenberg *et al.* 1999 Male Mouse – 600 ppm TCE 4 hour Inhalation



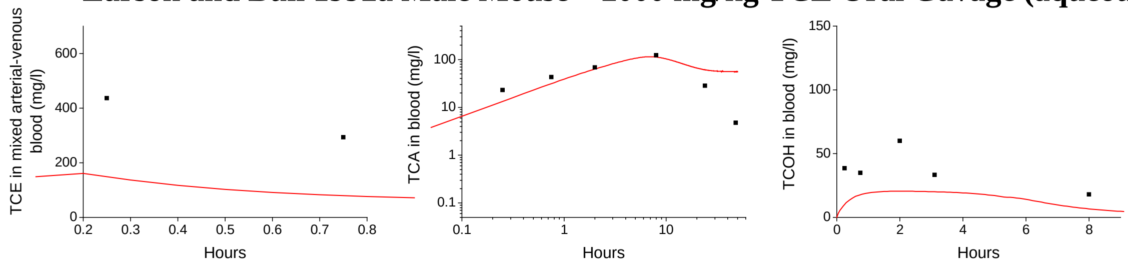
Greenberg *et al.* 1999 Male Mouse – 600 ppm TCE 4 hour Inhalation



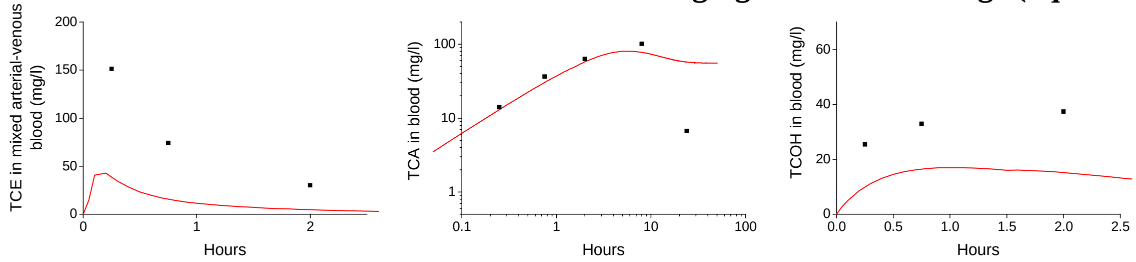
Larson and Bull 1992a Male Mouse – 197 mg/kg TCE Oral Gavage (aqueous)



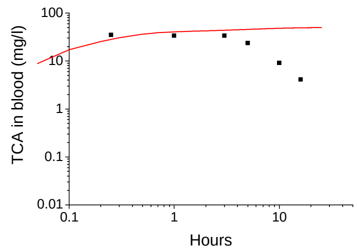
Larson and Bull 1992a Male Mouse – 2000 mg/kg TCE Oral Gavage (aqueous)



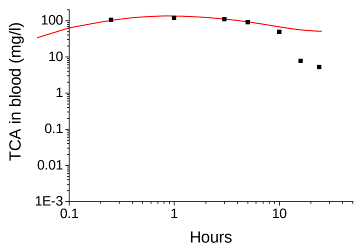
Larson and Bull 1992a Male Mouse – 592 mg/kg TCE Oral Gavage (aqueous)



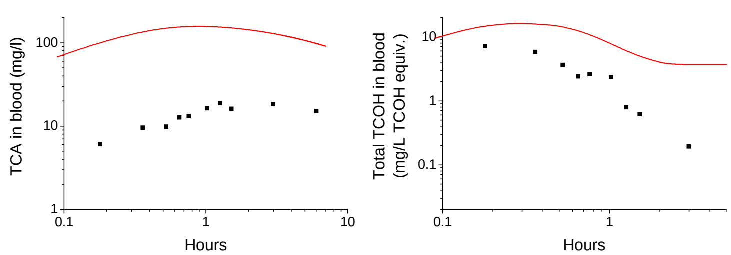
Larson and Bull 1992b Male Mouse – 20 mg/kg TCA Oral Gavage (aqueous)



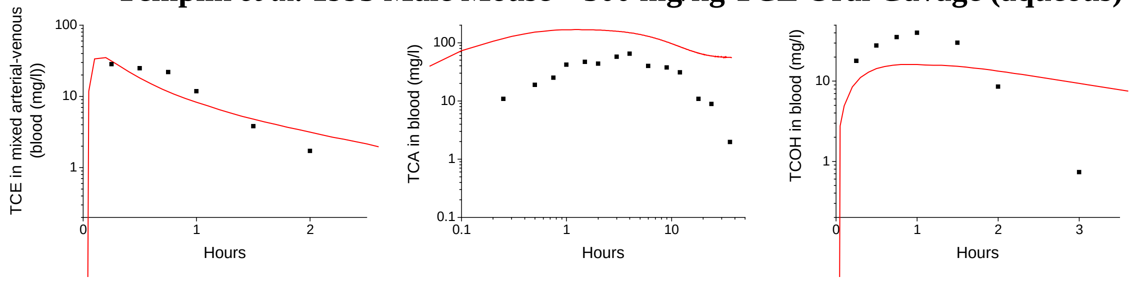
Larson and Bull 1992b Male Mouse – 100 mg/kg TCA Oral Gavage (aqueous)



Merdink *et al.* 1998 Male Mouse – 100 mg/kg TCE Intravenous



Templin *et al.* 1993 Male Mouse – 500 mg/kg TCE Oral Gavage (aqueous)



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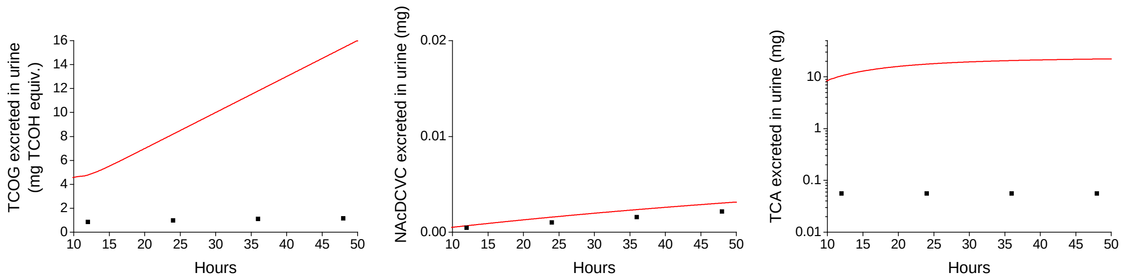
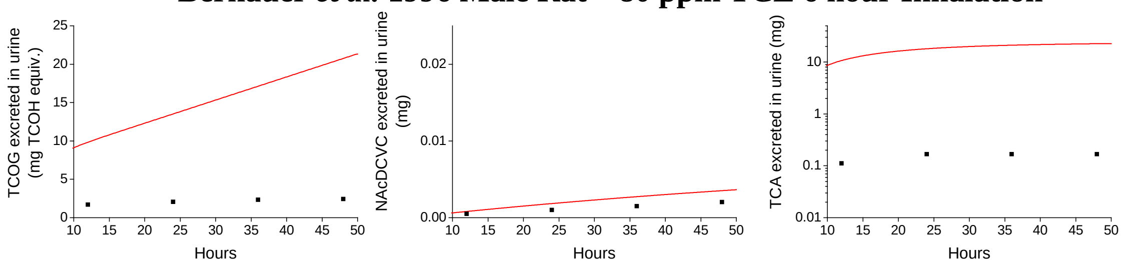
APPENDIX B. RAT VALIDATION FIGURES

Rat figures correspond to Figure A-32 in Appendix A of EPA (2011). Red lines represent model simulation using posterior population means. Citations for the original studies are in the Section 9.0 of the main report.

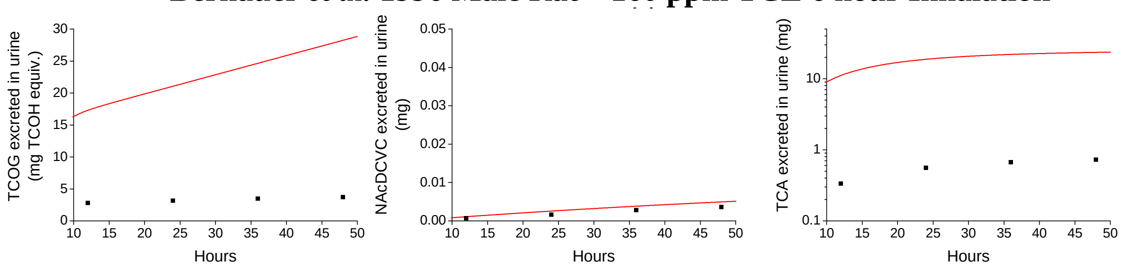
Bernauer *et al.* 1996 Male Rat – 40 ppm TCE 6 hour Inhalation



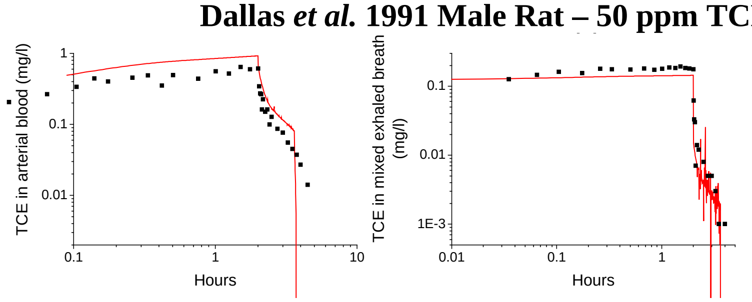
Bernauer *et al.* 1996 Male Rat – 80 ppm TCE 6 hour Inhalation



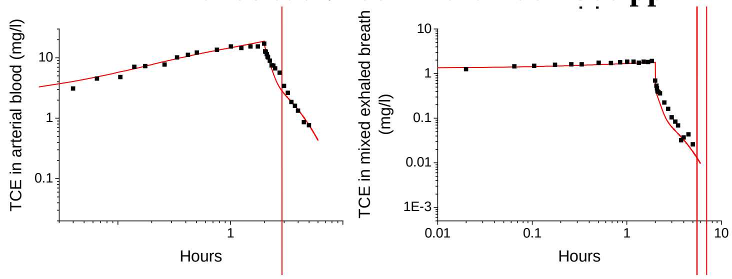
Bernauer *et al.* 1996 Male Rat – 160 ppm TCE 6 hour Inhalation



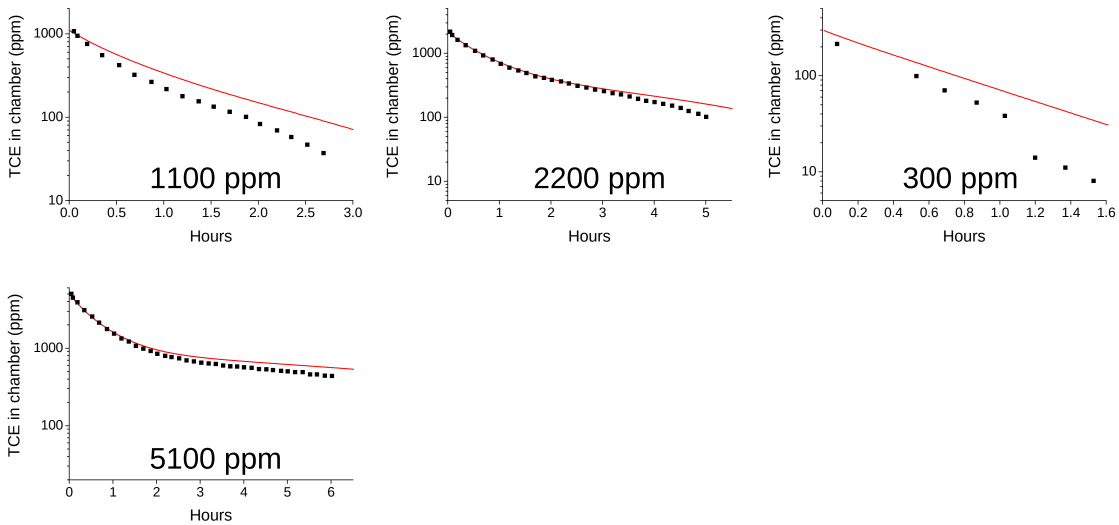
Dallas *et al.* 1991 Male Rat – 50 ppm TCE 2 hour Inhalation



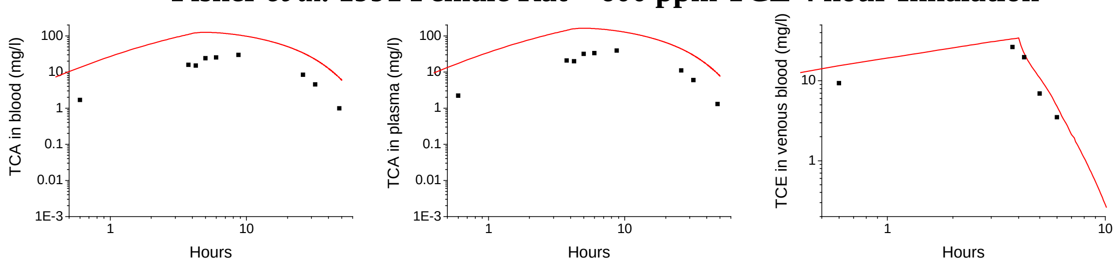
Dallas *et al.* 1991 Male Rat – 500 ppm TCE 2 hour Inhalation



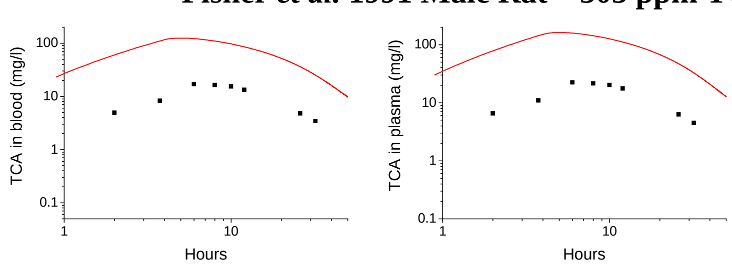
Fisher *et al.* 1989 Female Rat – TCE Closed Chamber



Fisher *et al.* 1991 Female Rat – 600 ppm TCE 4 hour Inhalation

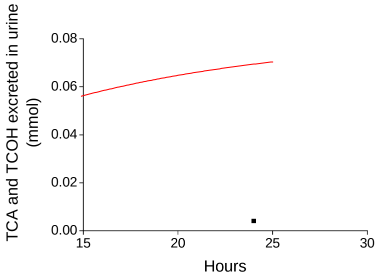


Fisher *et al.* 1991 Male Rat – 505 ppm TCE 4 hour Inhalation

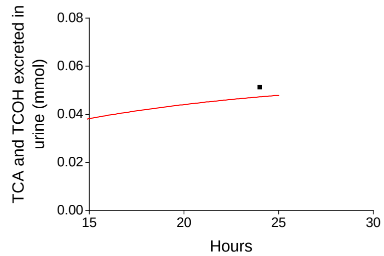


Green *et al.* 1985 Male Rat – TCA

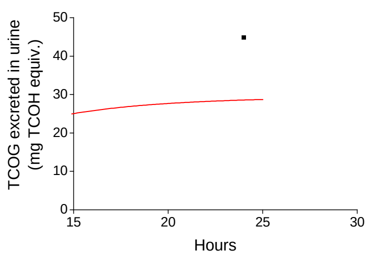
10 mg/kg intravenous

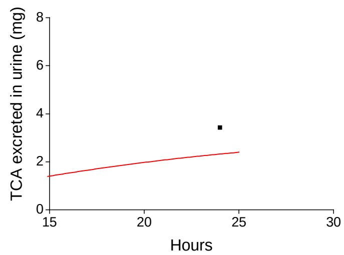


75 mg/kg Oral gavage (aqueous)

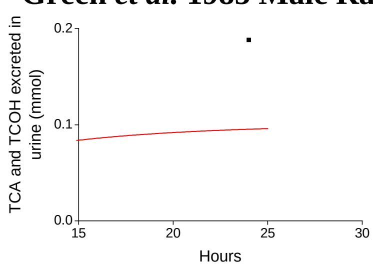


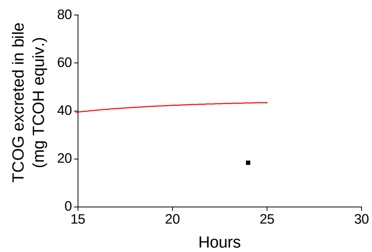
Green *et al.* 1985 Male Rat – 500 mg/kg TCE Oral Gavage (oil vehicle)



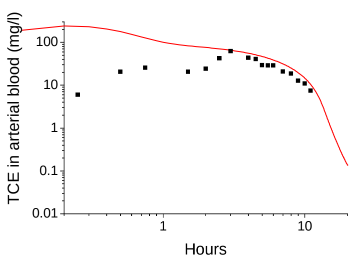


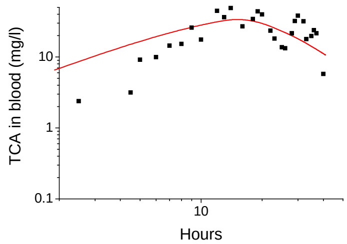
Green *et al.* 1985 Male Rat – 500 mg/kg TCE Oral Gavage (oil vehicle; bile cannulated)

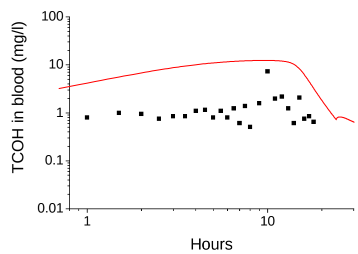




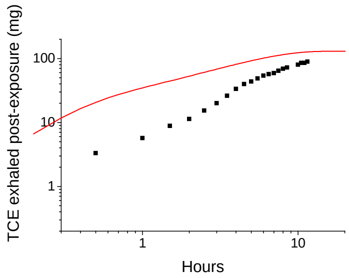
Prout *et al.* 1985 Male Rat – 1000 mg/kg TCE Oral Gavage (oil vehicle)



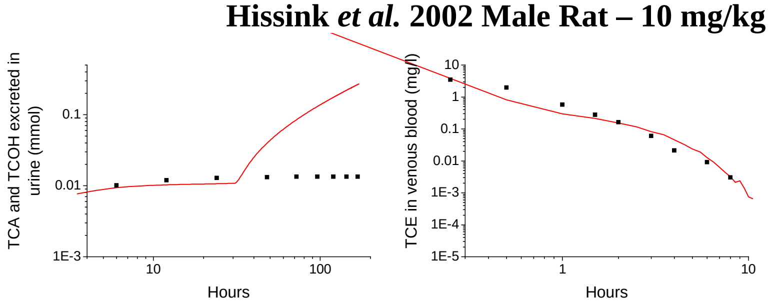




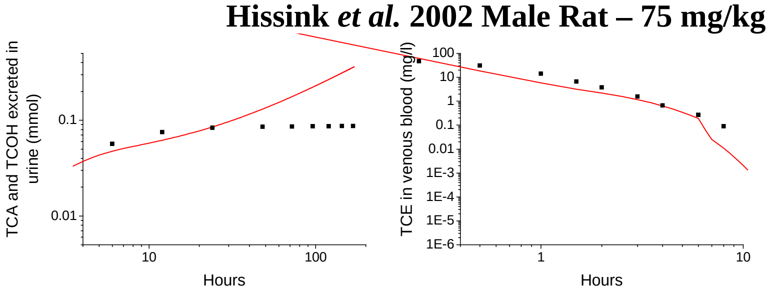
Prout *et al.* 1985 Male Rat – 1000 mg/kg TCE Oral Gavage (oil vehicle)



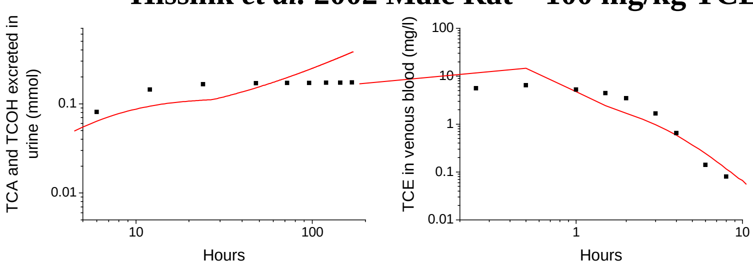
Hissink *et al.* 2002 Male Rat – 10 mg/kg TCE Intravenous



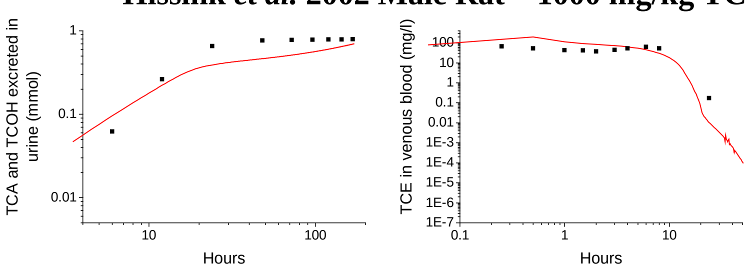
Hissink *et al.* 2002 Male Rat – 75 mg/kg TCE Intravenous



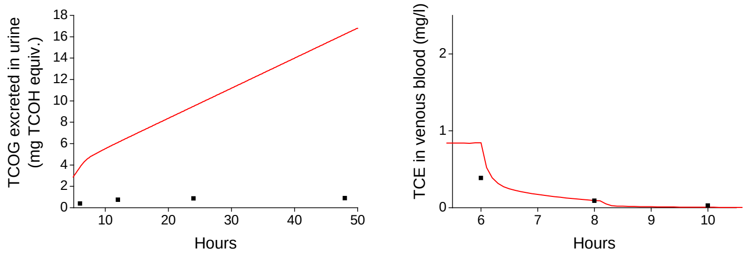
Hissink *et al.* 2002 Male Rat – 100 mg/kg TCE Oral Gavage (oil vehicle)



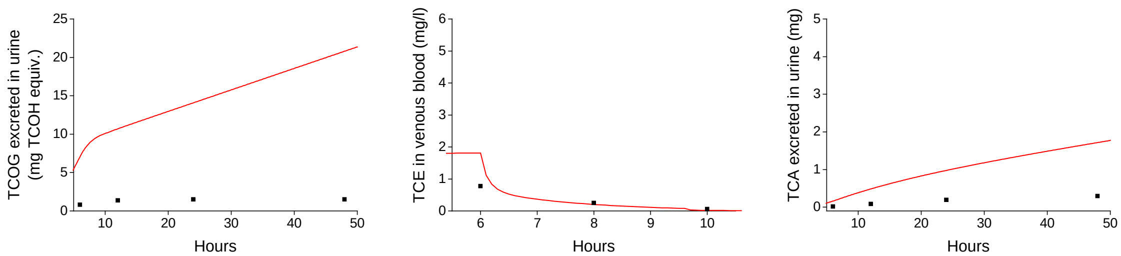
Hissink *et al.* 2002 Male Rat – 1000 mg/kg TCE Oral Gavage (oil vehicle)



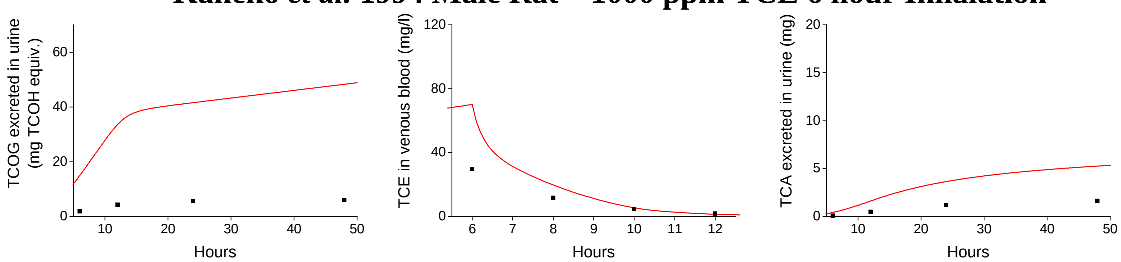
Kaneko *et al.* 1994 Male Rat – 50 ppm TCE 6 hour Inhalation



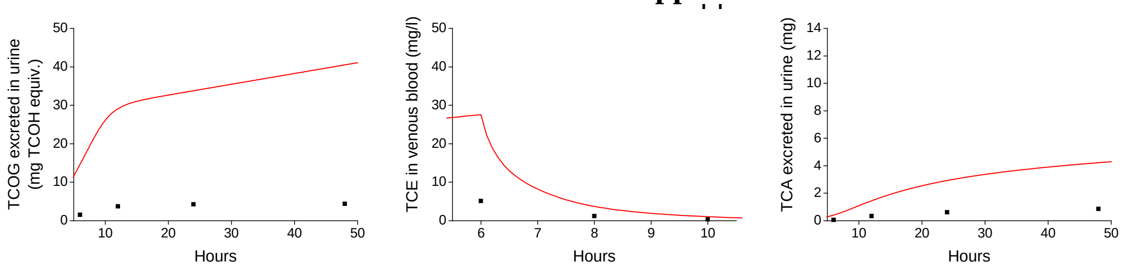
Kaneko *et al.* 1994 Male Rat – 100 ppm TCE 6 hour Inhalation



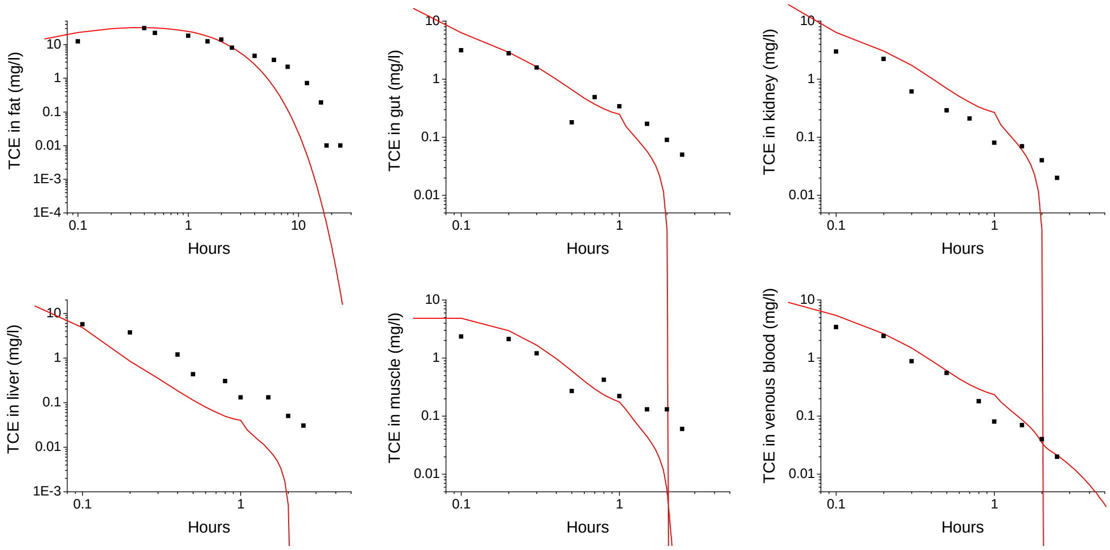
Kaneko *et al.* 1994 Male Rat – 1000 ppm TCE 6 hour Inhalation



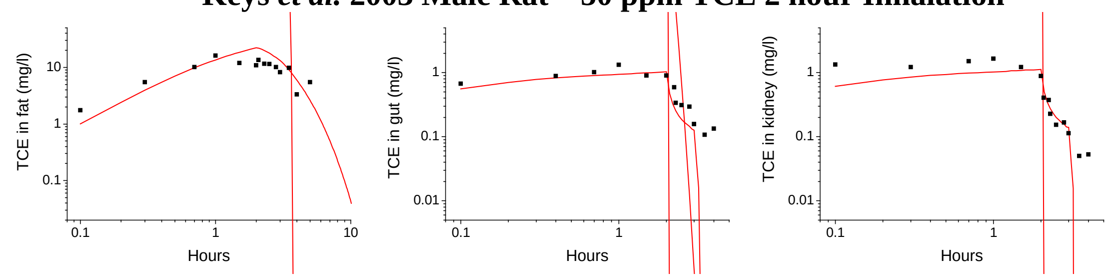
Kaneko *et al.* 1994 Male Rat – 500 ppm TCE 6 hour Inhalation



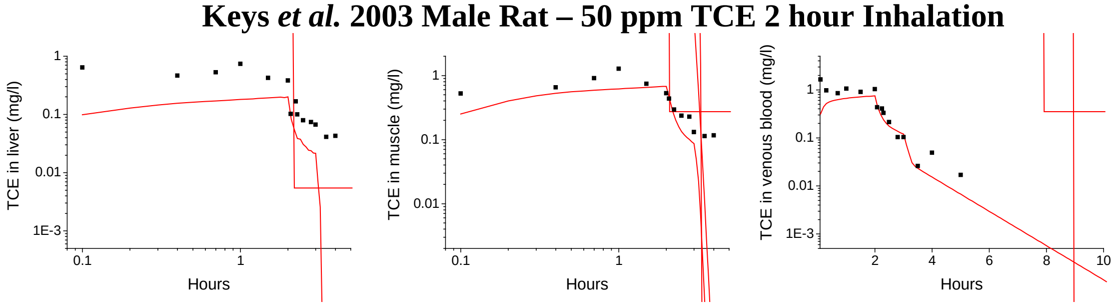
Keys *et al.* 2003 Male Rat – 8 mg/kg TCE Intra-arterial



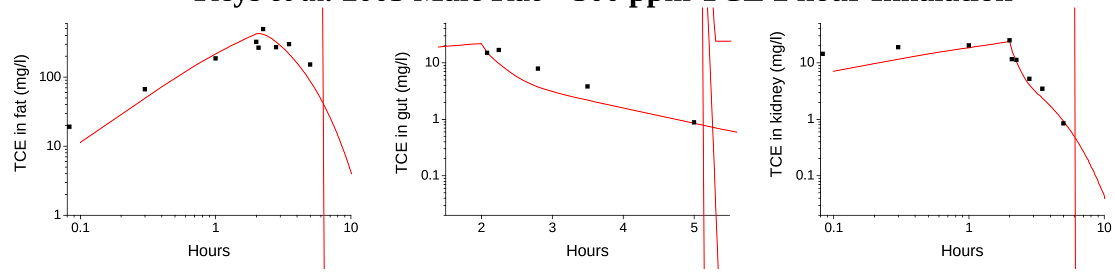
Keys *et al.* 2003 Male Rat – 50 ppm TCE 2 hour Inhalation



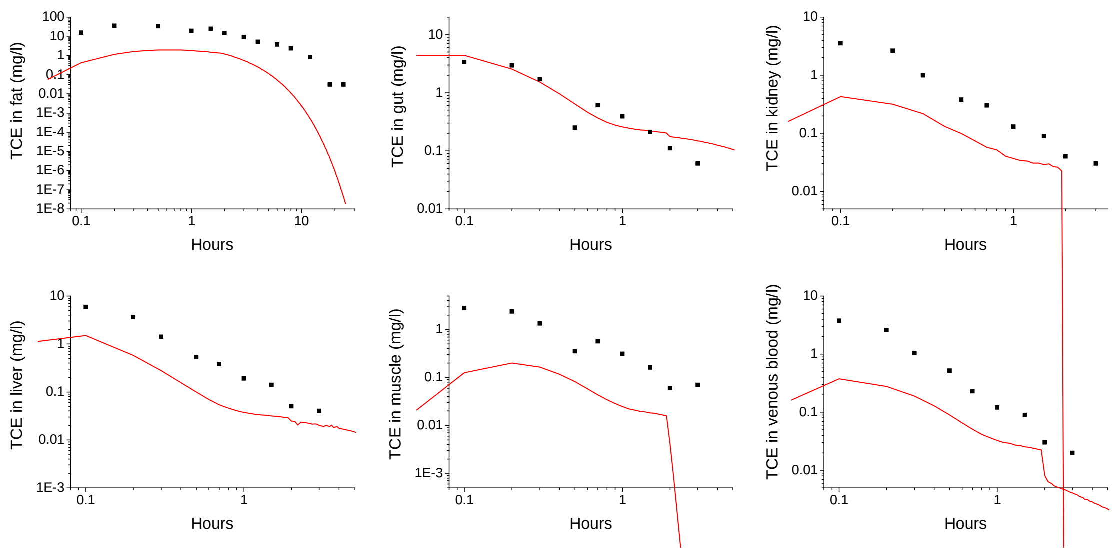
Keys *et al.* 2003 Male Rat – 50 ppm TCE 2 hour Inhalation



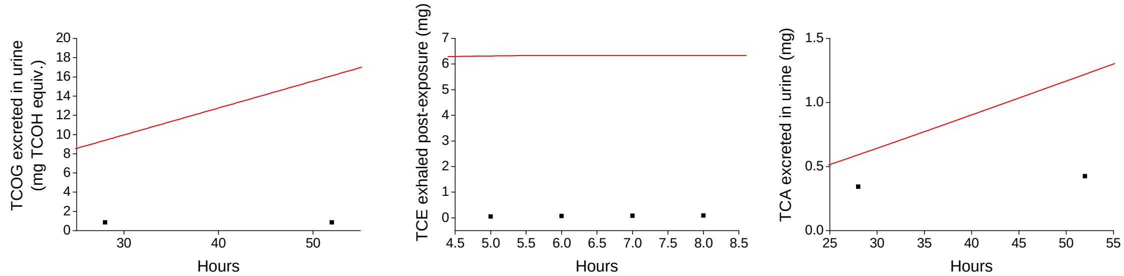
Keys *et al.* 2003 Male Rat – 500 ppm TCE 2 hour Inhalation



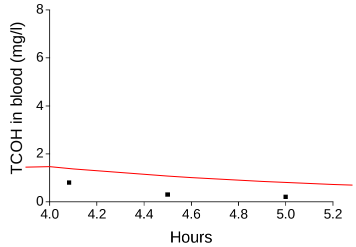
Keys *et al.* 2003 Male Rat – 8 mg/kg TCE Oral Gavage (aqueous)



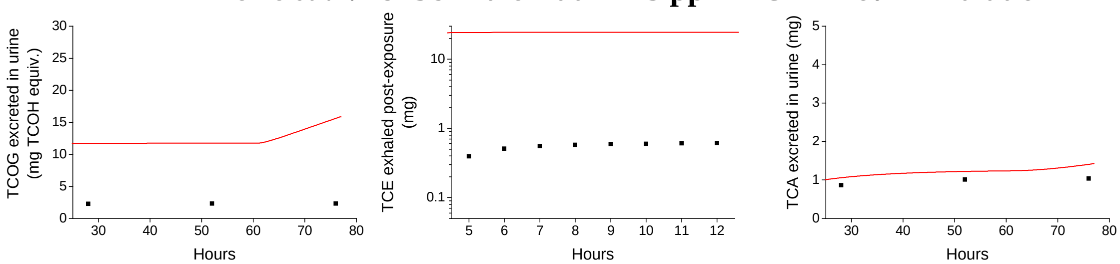
Kimmerle *et al.* 1973b Male Rat – 49 ppm TCE 4 hour Inhalation



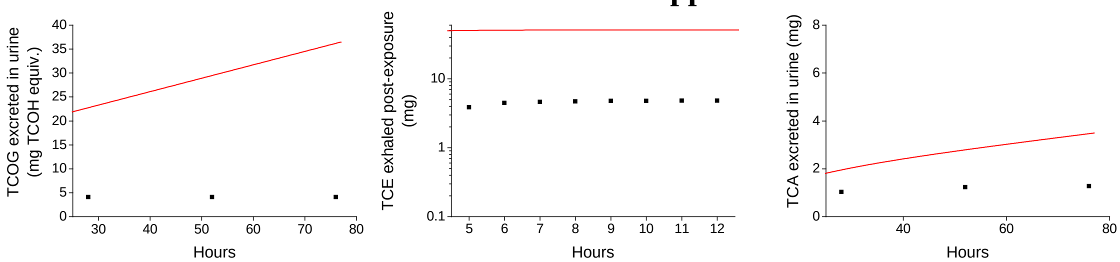
Kimmerle *et al.* 1973b Male Rat – 54 ppm TCE 4 hour Inhalation



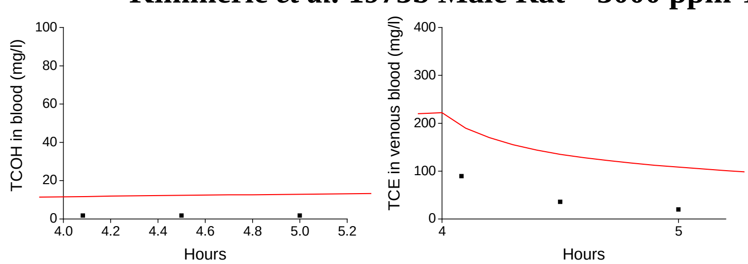
Kimmerle *et al.* 1973b Male Rat – 175 ppm TCE 4 hour Inhalation



Kimmerle *et al.* 1973b Male Rat – 330 ppm TCE 4 hour Inhalation

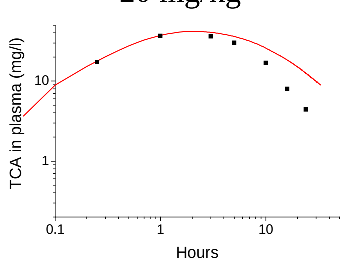


Kimmerle *et al.* 1973b Male Rat – 3000 ppm TCE 4 hour Inhalation

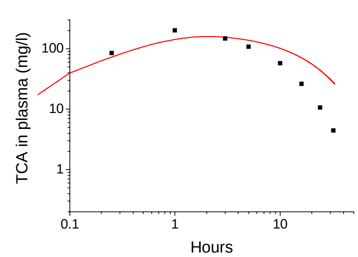


Larson and Bull 1992a Male Rat – TCA Oral Gavage (aqueous)

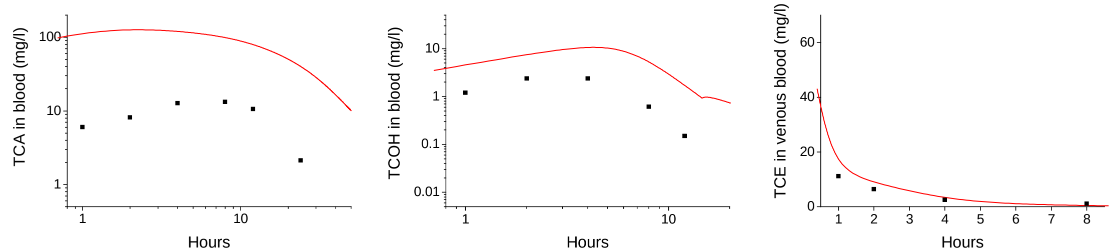
20 mg/kg



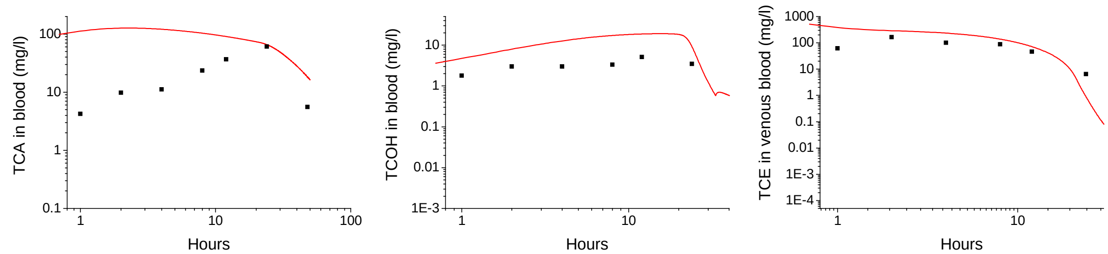
100 mg/kg



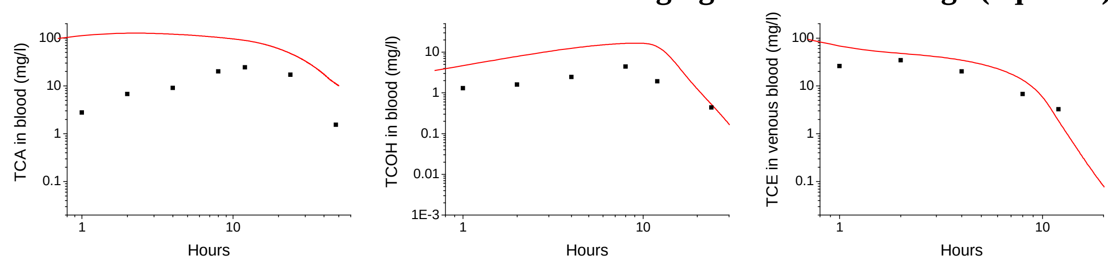
Larson and Bull 1992b Male Rat – 197 mg/kg TCE Oral Gavage (aqueous)



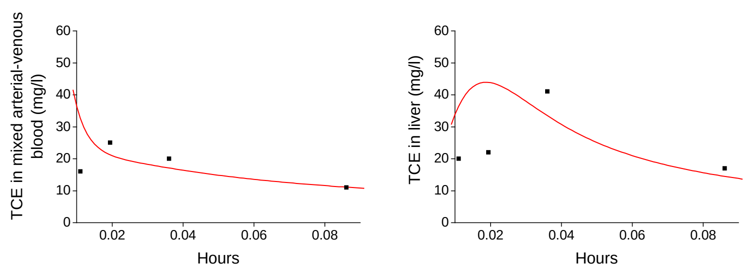
Larson and Bull 1992b Male Rat – 3000 mg/kg TCE Oral Gavage (aqueous)



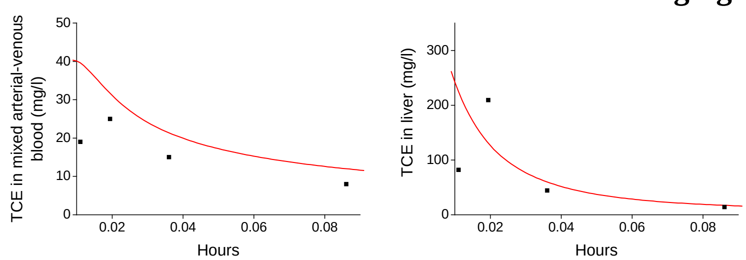
Larson and Bull 1992b Male Rat – 592 mg/kg TCE Oral Gavage (aqueous)



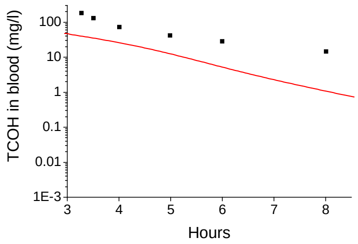
Lee *et al.* 2000 Male Rat – 16 mg/kg TCE Intravenous



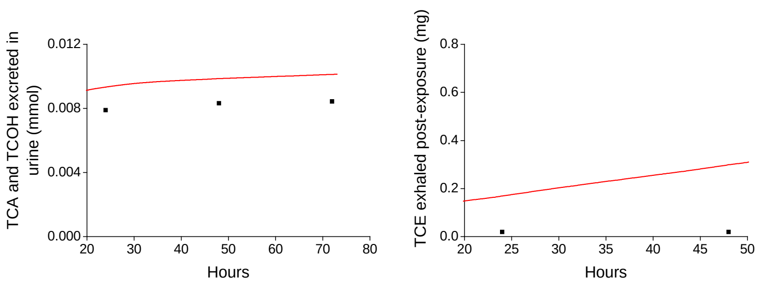
Lee *et al.* 2000 Male Rat – 16 mg/kg TCE Intravenous



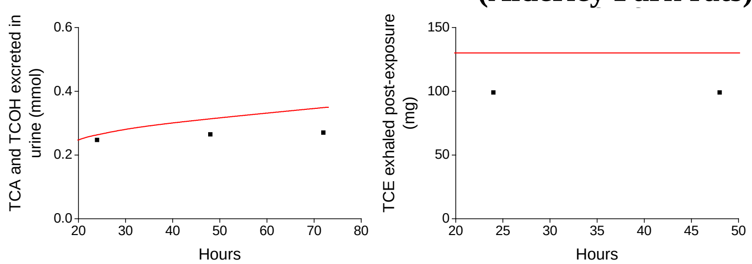
Merdink *et al.* 1999 Male Rat – 100 mg/kg TCOH Intravenous (aqueous)



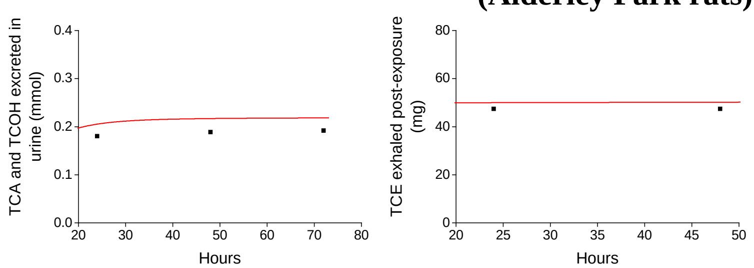
Prout *et al.* 1985 Male Rat – 10 mg/kg TCE Oral Gavage (oil vehicle) (Alderley Park rats)



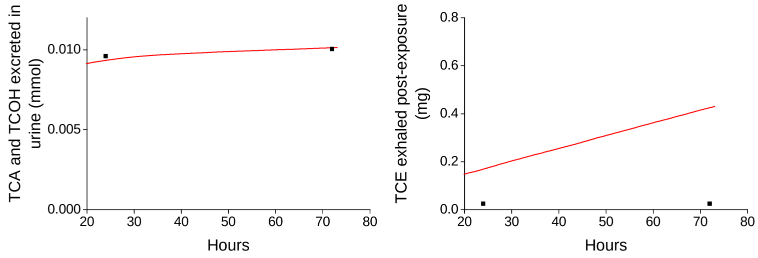
Prout *et al.* 1985 Male Rat – 1000 mg/kg TCE Oral Gavage (oil vehicle) (Alderley Park rats)



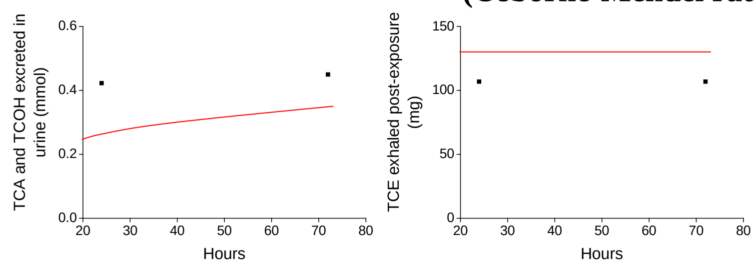
Prout *et al.* 1985 Male Rat – 500 mg/kg TCE Oral Gavage (oil vehicle) (Alderley Park rats)



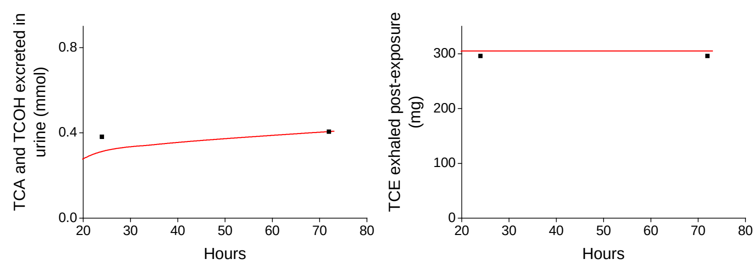
Prout *et al.* 1985 Male Rat – 10 mg/kg TCE Oral Gavage (oil vehicle) (Osborne-Mendel rats)



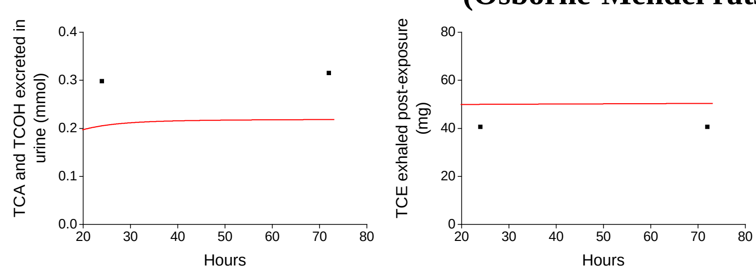
Prout *et al.* 1985 Male Rat – 1000 mg/kg TCE Oral Gavage (oil vehicle) (Osborne-Mendel rats)



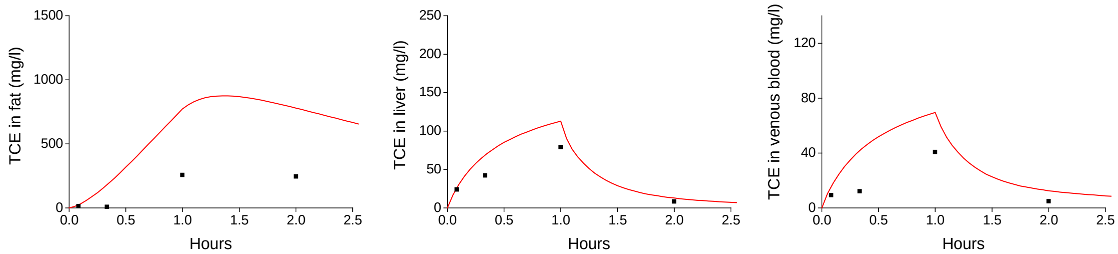
Prout *et al.* 1985 Male Rat – 2000 mg/kg TCE Oral Gavage (oil vehicle) (Osborne-Mendel rats)



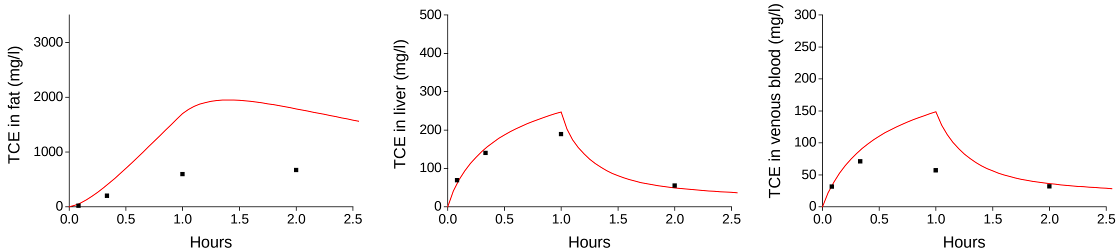
Prout *et al.* 1985 Male Rat – 500 mg/kg TCE Oral Gavage (oil vehicle) (Osborne-Mendel rats)



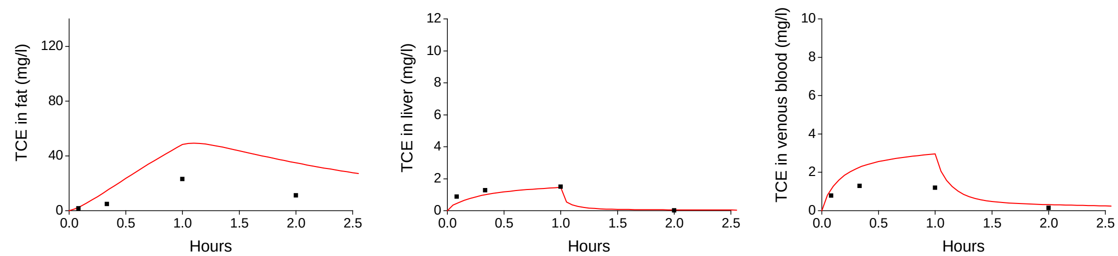
Simmons *et al.* 2002 Male Rat – 2000 ppm TCE 1 hour Inhalation



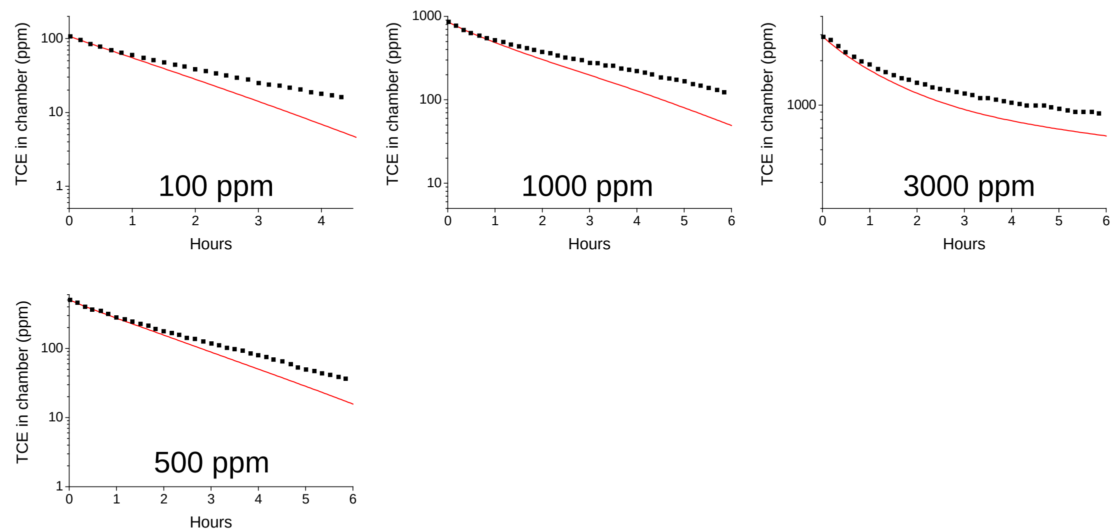
Simmons *et al.* 2002 Male Rat – 4000 ppm TCE 1 hour Inhalation



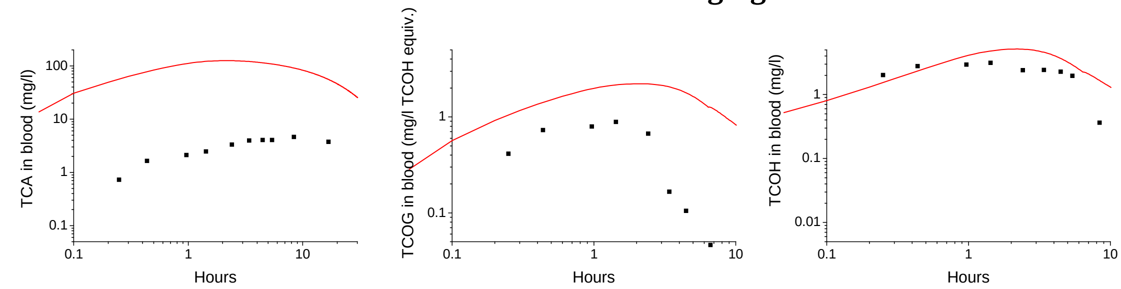
Simmons *et al.* 2002 Male Rat – 200 ppm TCE 1 hour Inhalation



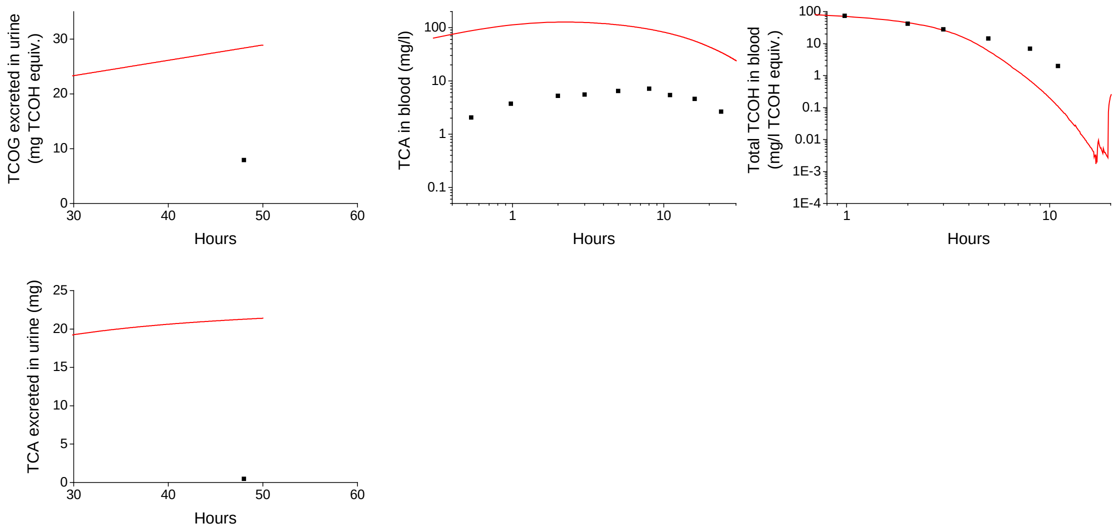
Simmons *et al.* 2002 Male Rat – TCE Closed Chamber



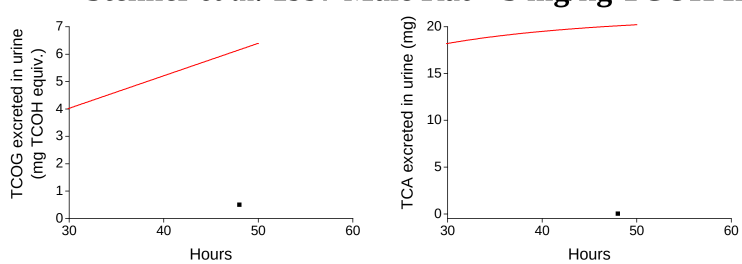
Stenner *et al.* 1997 Male Rat – 100 mg/kg TCE Intravenous



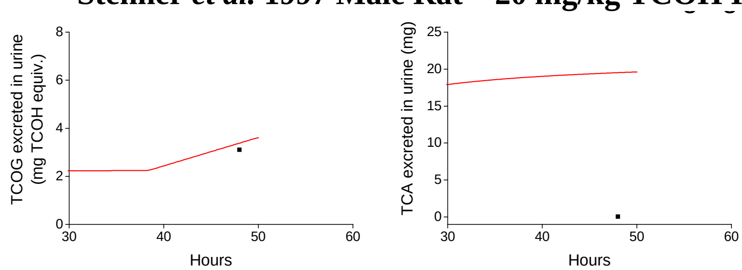
Stenner *et al.* 1997 Male Rat – 100 mg/kg TCOH Intravenous



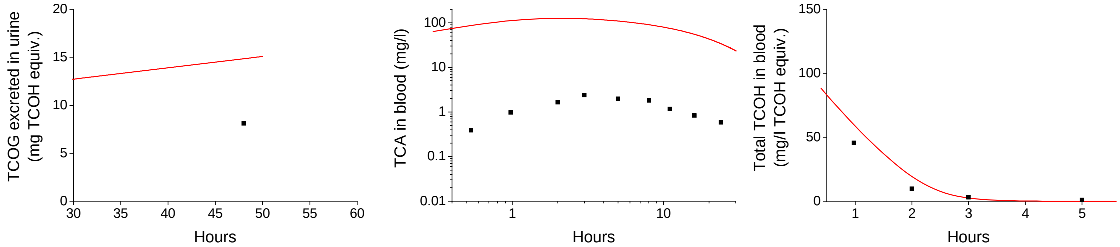
Stenner *et al.* 1997 Male Rat – 5 mg/kg TCOH Intravenous (bile cannulated)



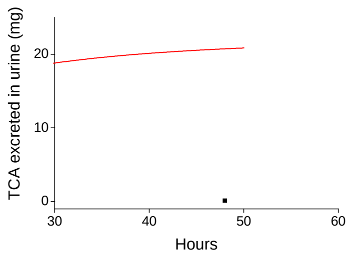
Stenner *et al.* 1997 Male Rat – 20 mg/kg TCOH Intravenous (bile cannulated)



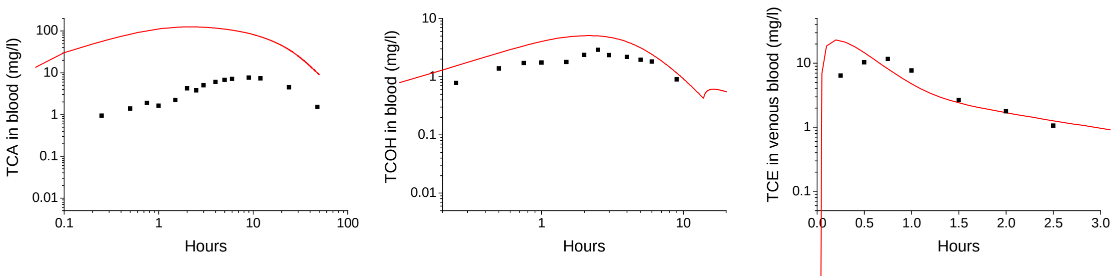
Stenner *et al.* 1997 Male Rat – 100 mg/kg TCOH Intravenous (bile cannulated)



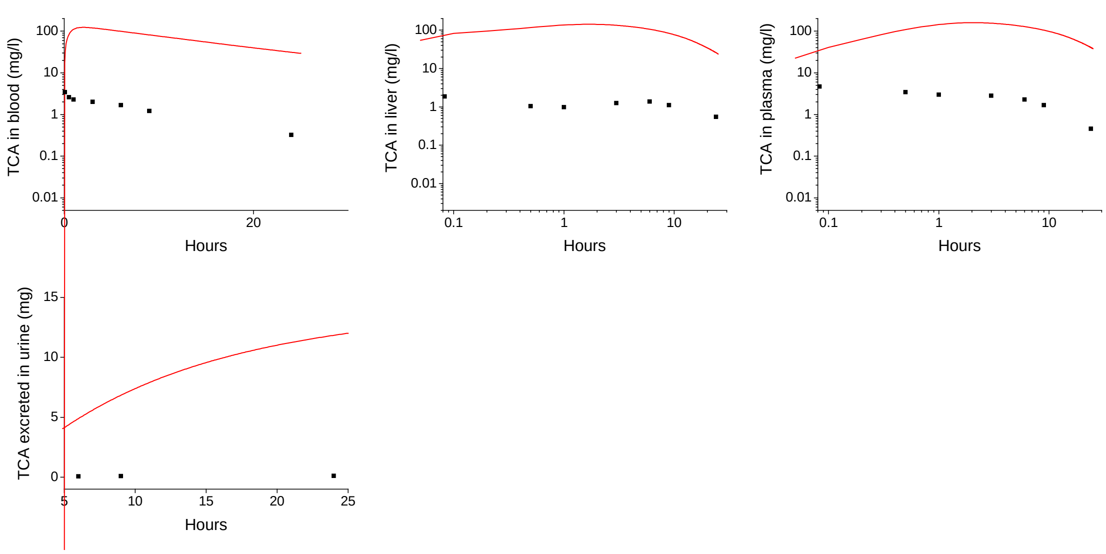
Stenner *et al.* 1997 Male Rat – 100 mg/kg TCOH Intravenous (bile cannulated)



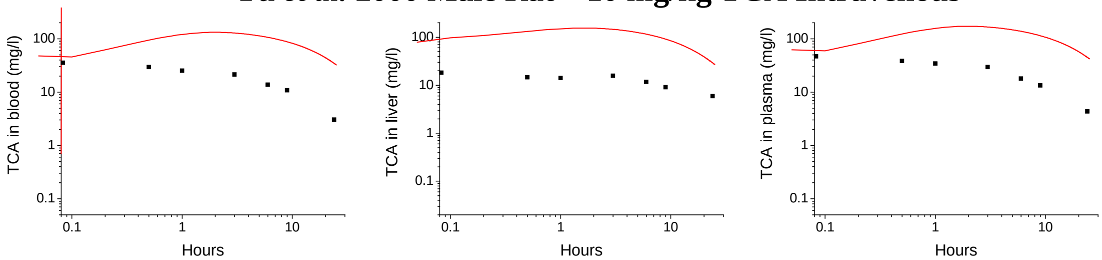
Templin *et al.* 1995 Male Rat – 100 mg/kg TCE Oral Gavage (aqueous)



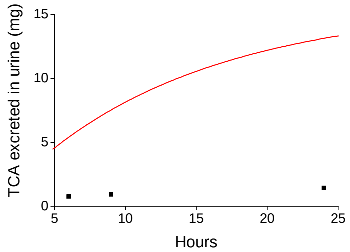
Yu *et al.* 2000 Male Rat – 1 mg/kg TCA Intravenous



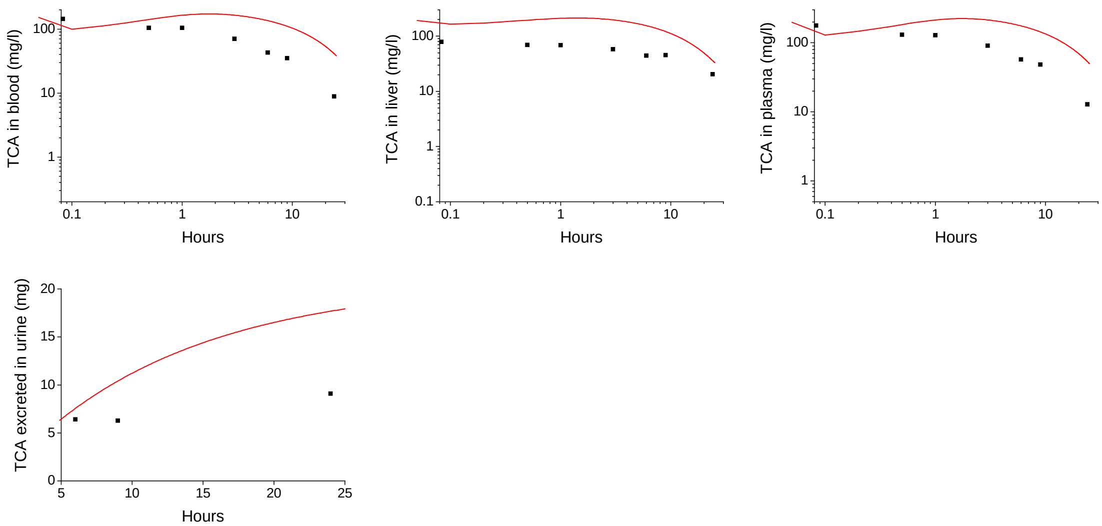
Yu *et al.* 2000 Male Rat – 10 mg/kg TCA Intravenous



Yu *et al.* 2000 Male Rat – 10 mg/kg TCA Intravenous



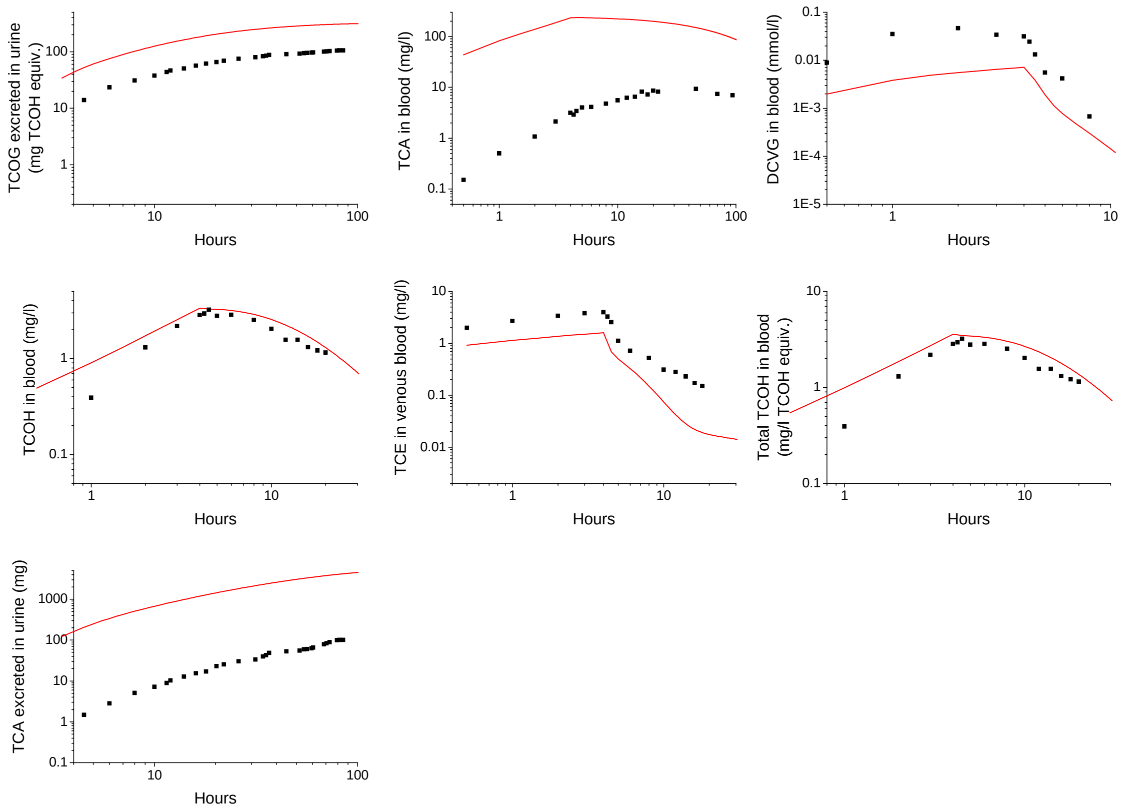
Yu *et al.* 2000 Male Rat – 50 mg/kg TCA Intravenous



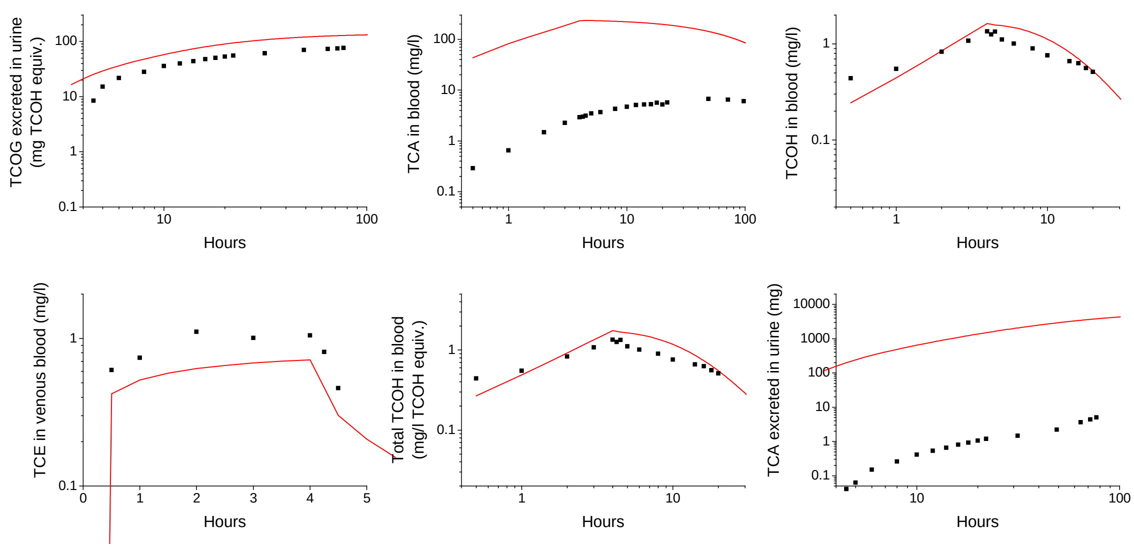
APPENDIX C. HUMAN VALIDATION FIGURES

Human figures correspond to Figure A-33 in Appendix A of EPA (2011). Red lines represent model simulation using posterior population means. Citations for the original studies are in the Section 9.0 of the main report.

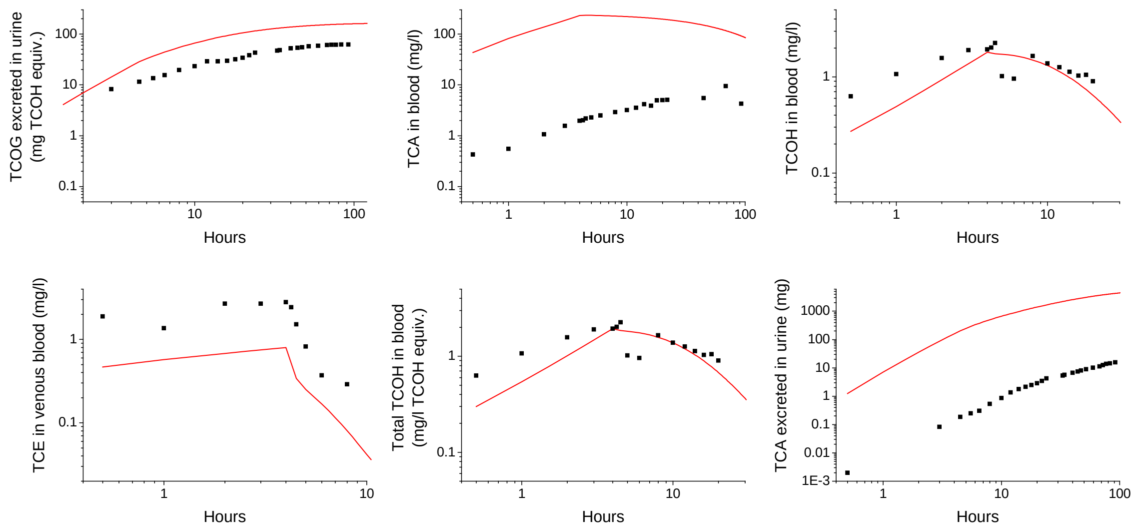
Fisher *et al.* 1998 Human #1 (sex=Male) – 105.5 ppm TCE 4 hour Inhalation



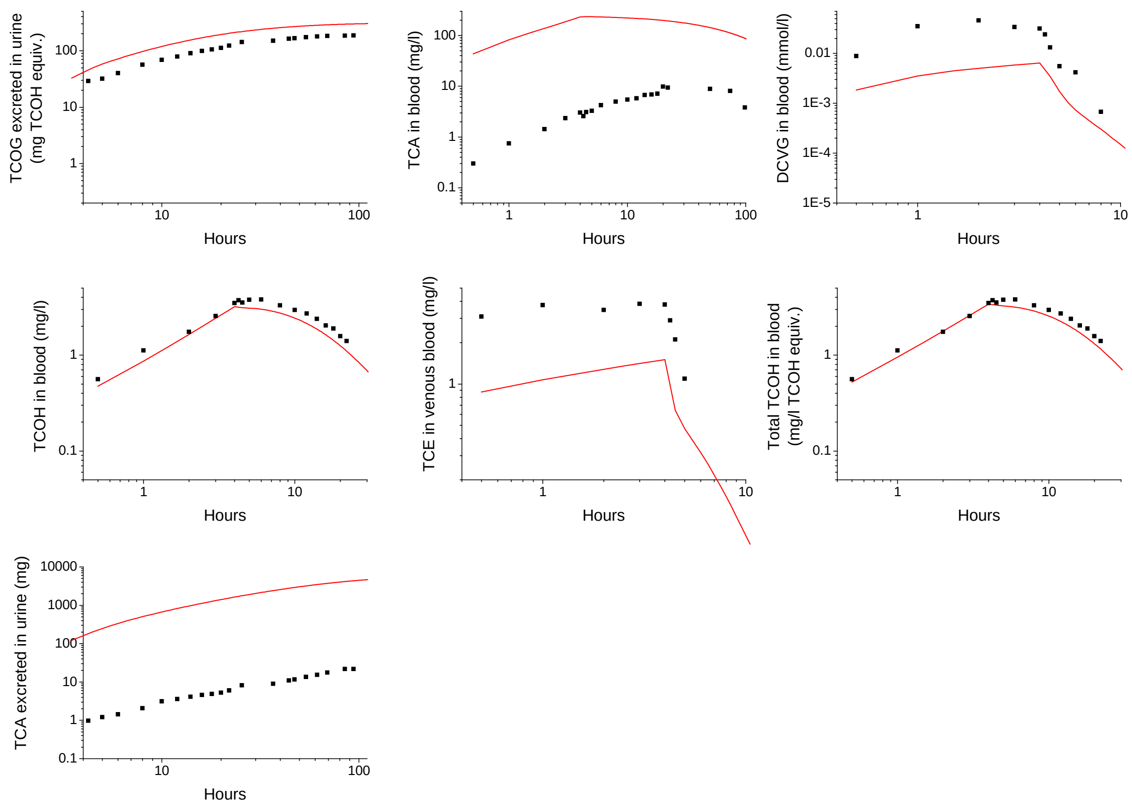
Fisher *et al.* 1998 Human #2 (sex=Male) – 49.3 ppm TCE 4 hour Inhalation



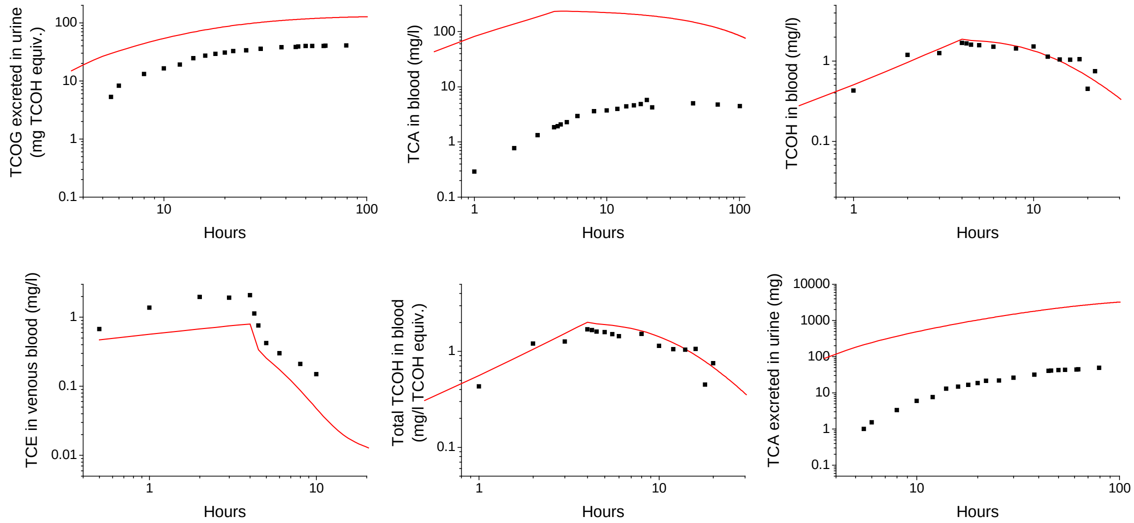
Fisher *et al.* 1998 Human #3 (sex=Male) – 55.2 ppm TCE 4 hour Inhalation



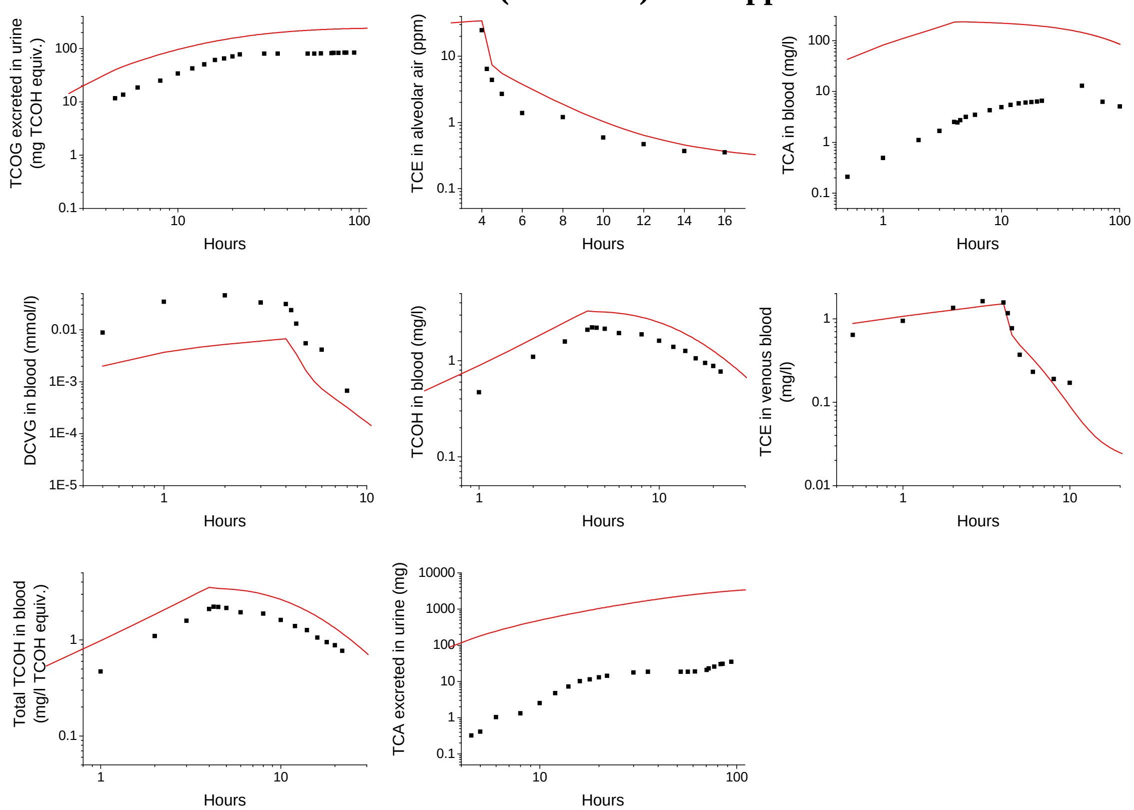
Fisher *et al.* 1998 Human #3 (sex=Male) – 101.5 ppm TCE 4 hour Inhalation



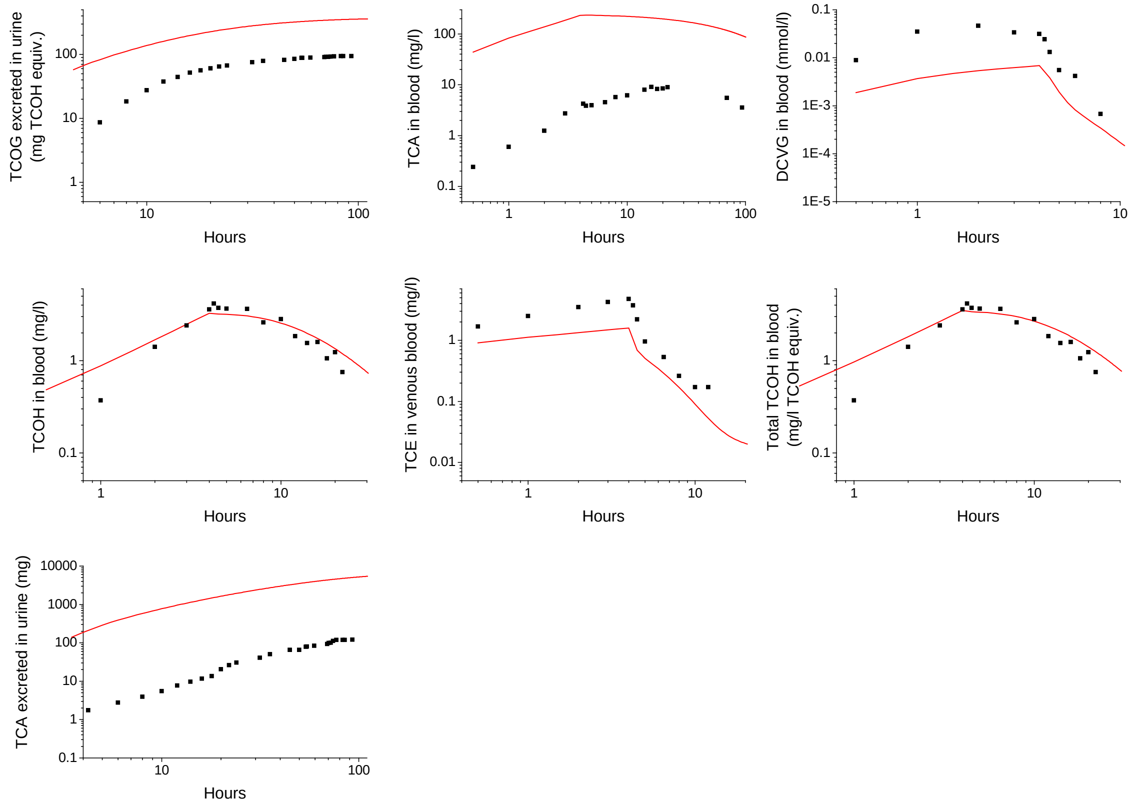
Fisher *et al.* 1998 Human #4 (sex=Male) – 53.1 ppm TCE 4 hour Inhalation



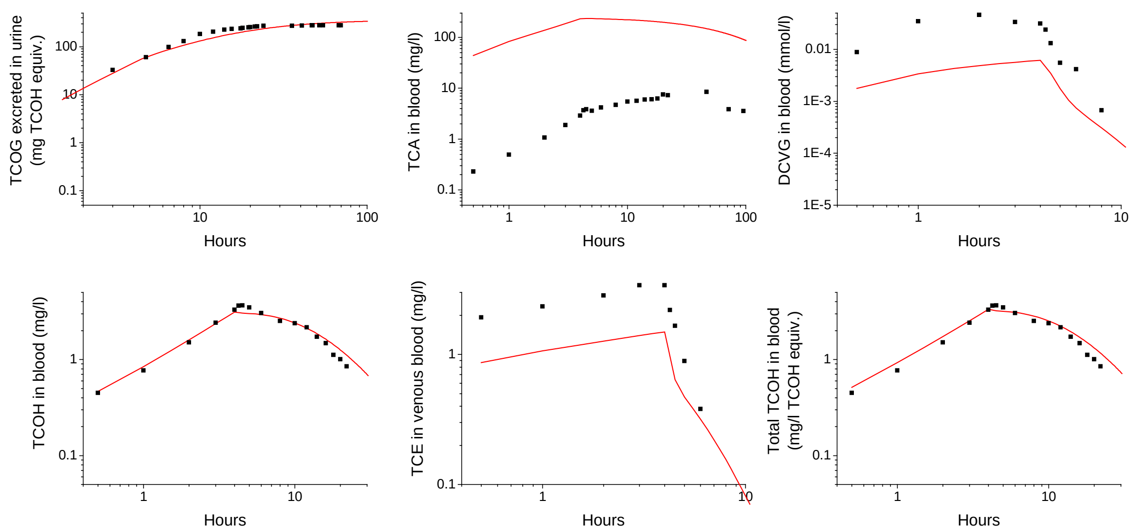
Fisher *et al.* 1998 Human #4 (sex=Male) – 97.8 ppm TCE 4 hour Inhalation



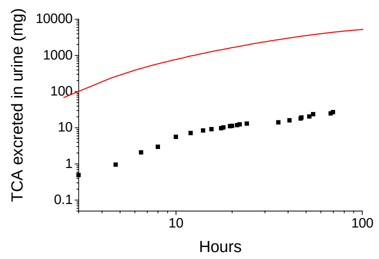
Fisher *et al.* 1998 Human #5 (sex=Male) – 105.5 ppm TCE 4 hour Inhalation



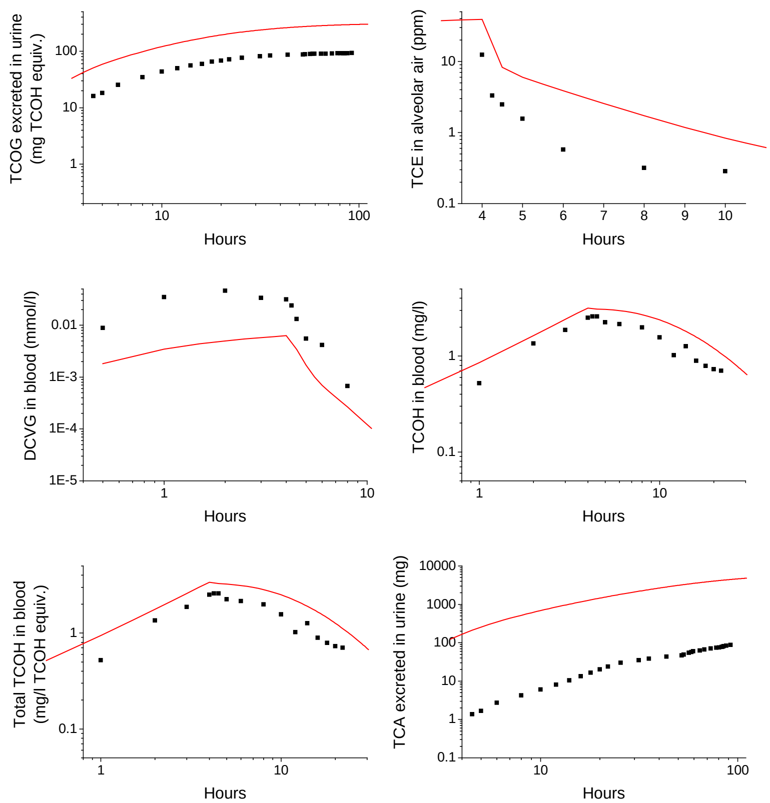
Fisher *et al.* 1998 Human #6 (sex=Male) – 102.6 ppm TCE 4 hour Inhalation



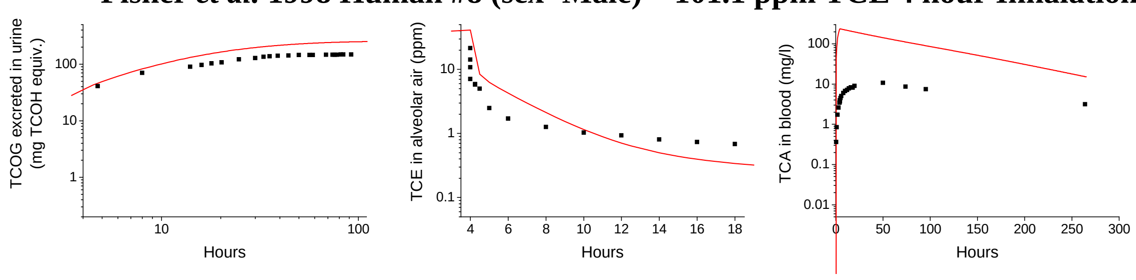
Fisher *et al.* 1998 Human #6 (sex=Male) – 102.6 ppm TCE 4 hour Inhalation



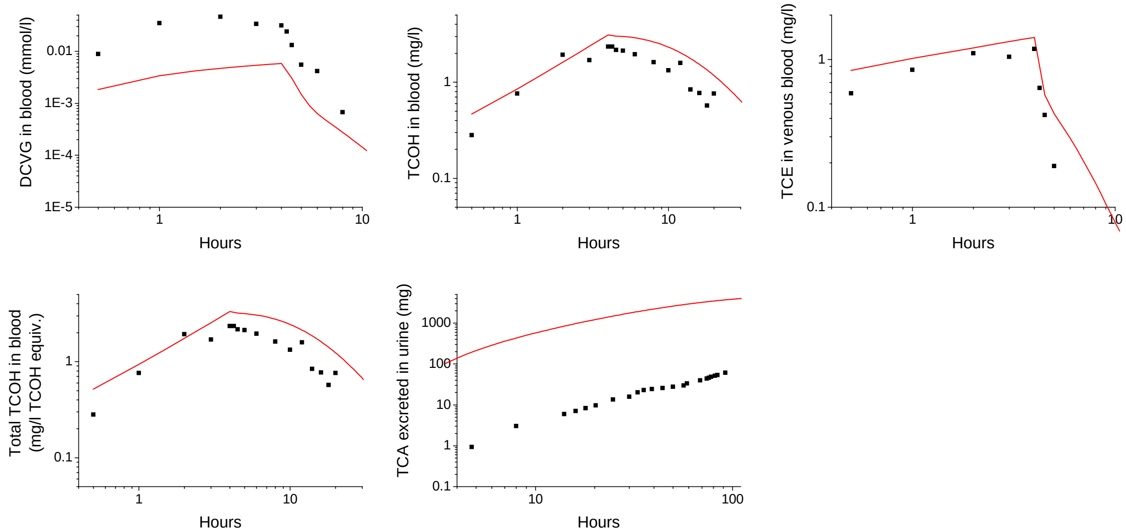
Fisher *et al.* 1998 Human #7 (sex=Male) – 102 ppm TCE 4 hour Inhalation



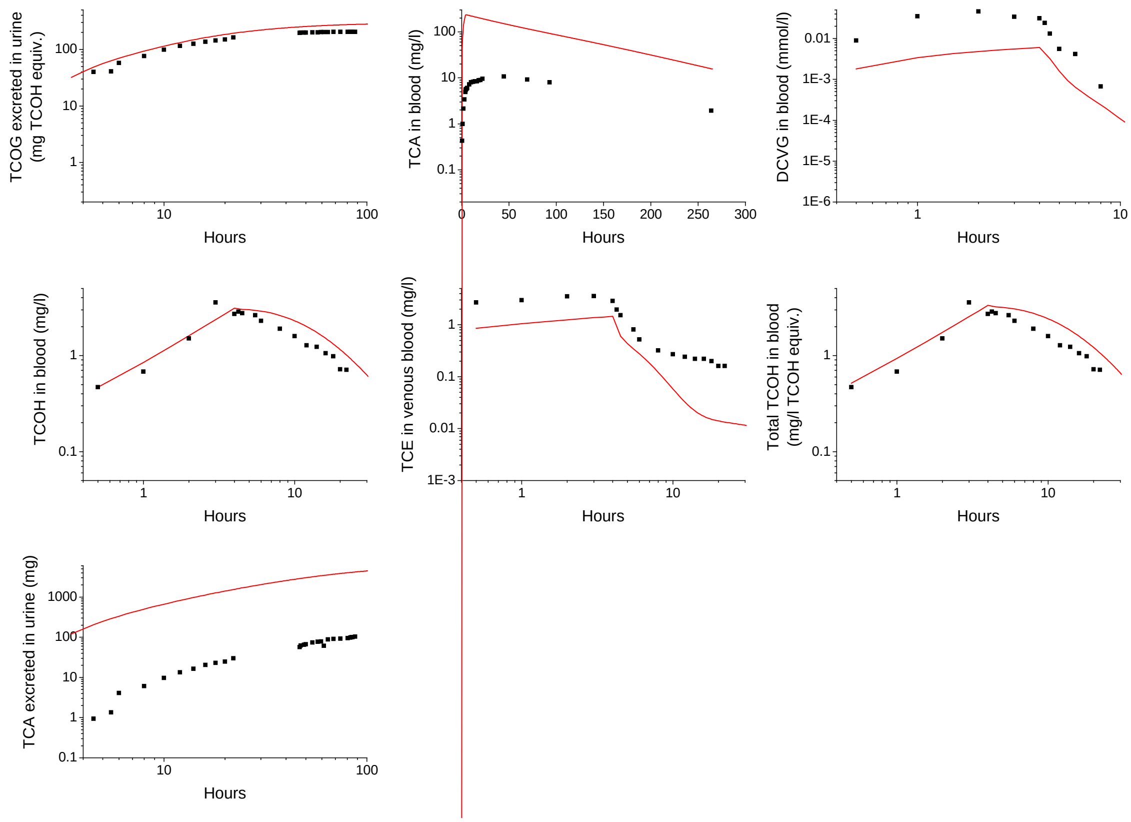
Fisher *et al.* 1998 Human #8 (sex=Male) – 101.1 ppm TCE 4 hour Inhalation



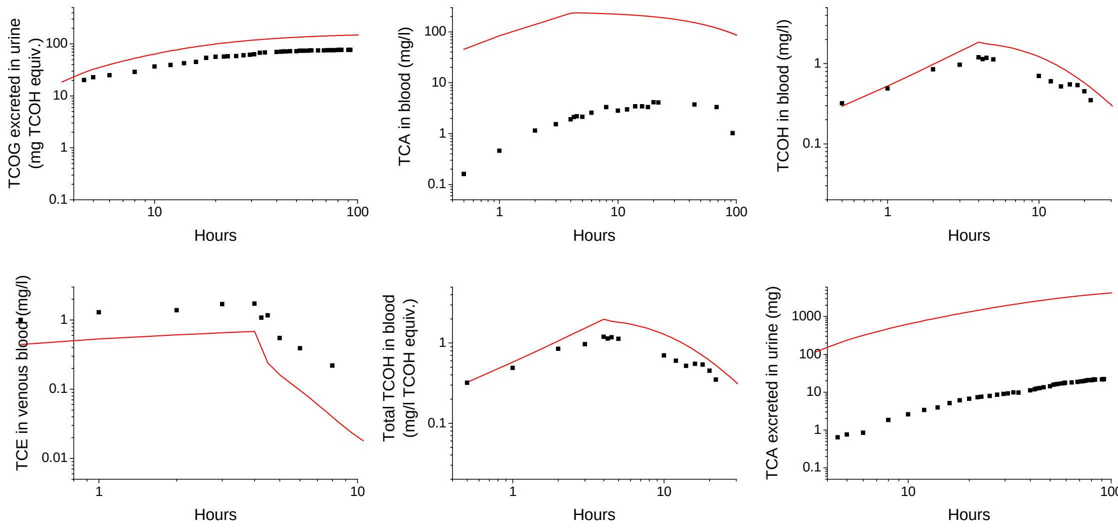
Fisher *et al.* 1998 Human #8 (sex=Male) – 101.1 ppm TCE 4 hour Inhalation



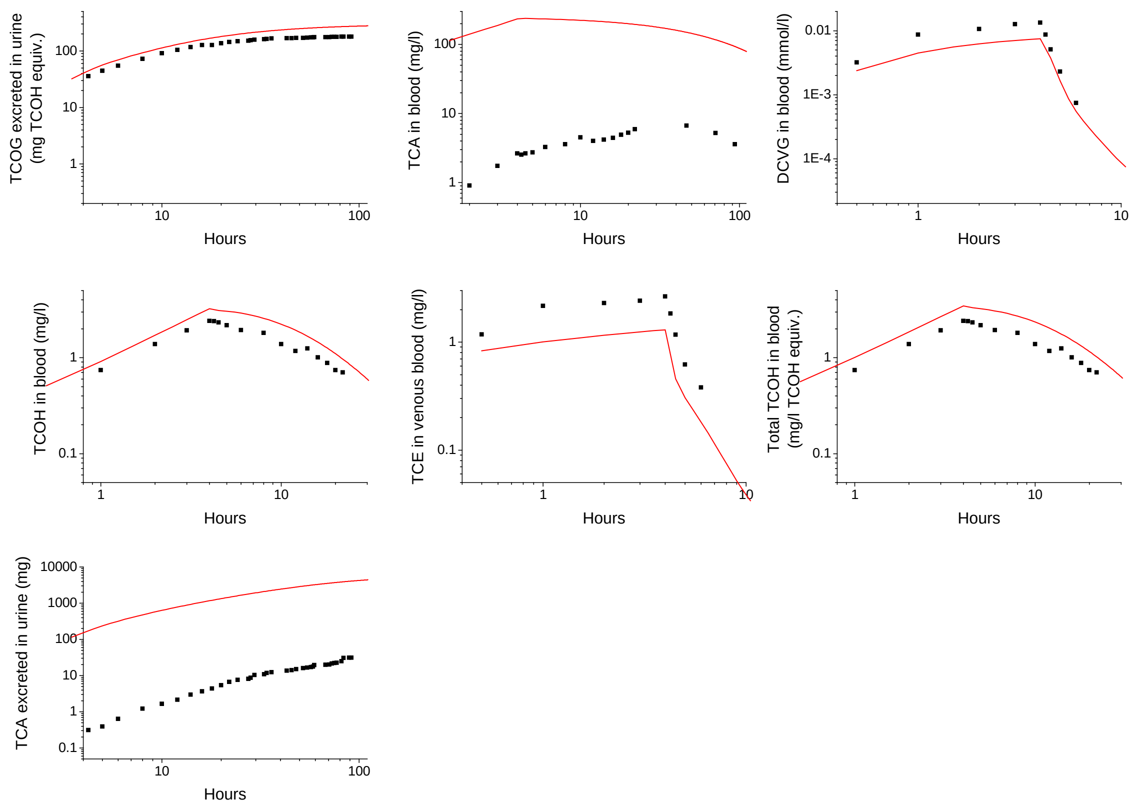
Fisher *et al.* 1998 Human #9 (sex=Male) – 103.4 ppm TCE 4 hour Inhalation



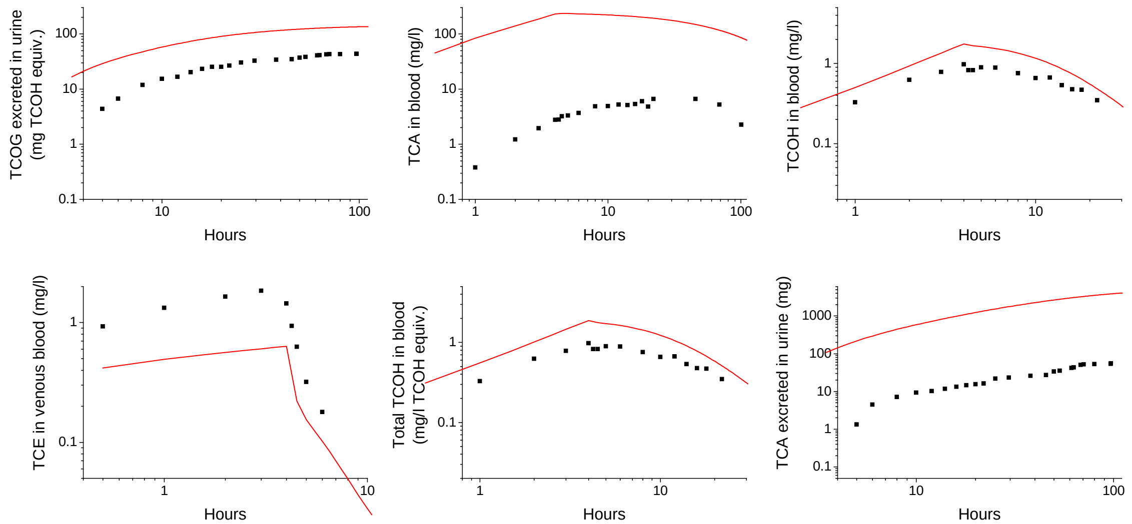
Fisher *et al.* 1998 Human #10 (sex=Female) – 55.1 ppm TCE 4 hour Inhalation



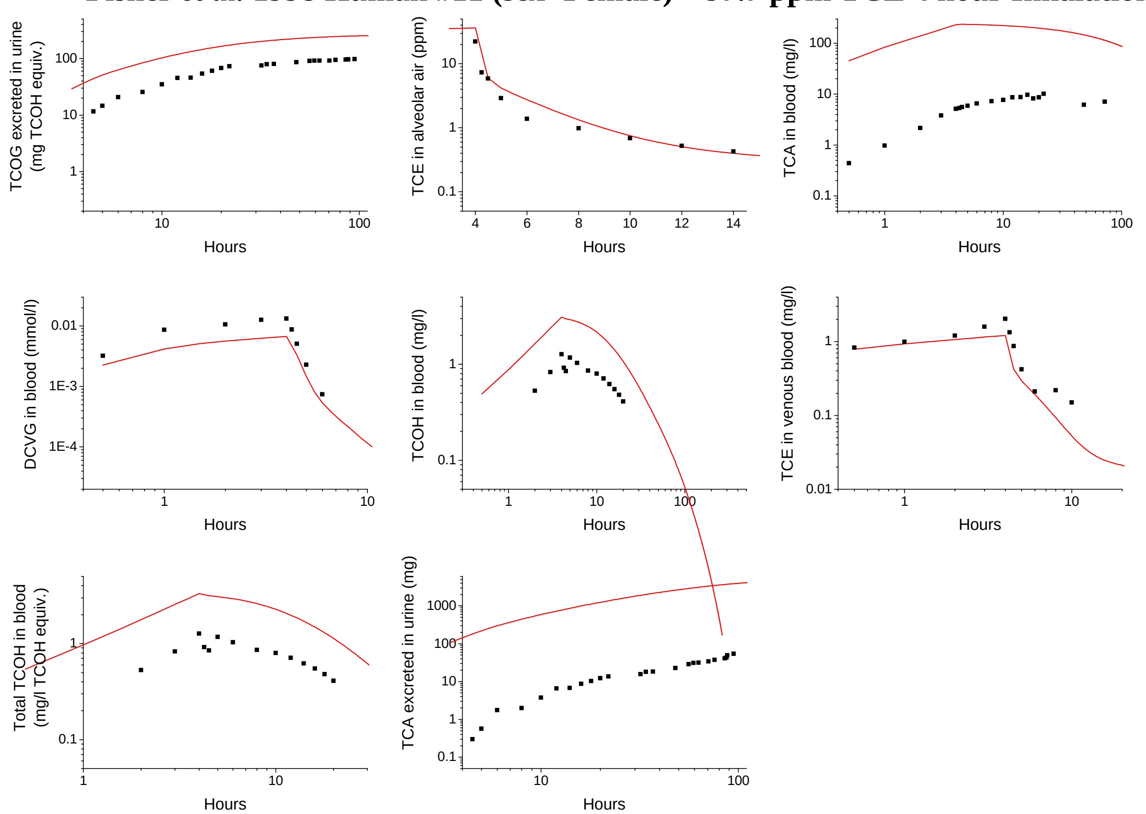
Fisher *et al.* 1998 Human #10 (sex=Female) – 101.4 ppm TCE 4 hour Inhalation



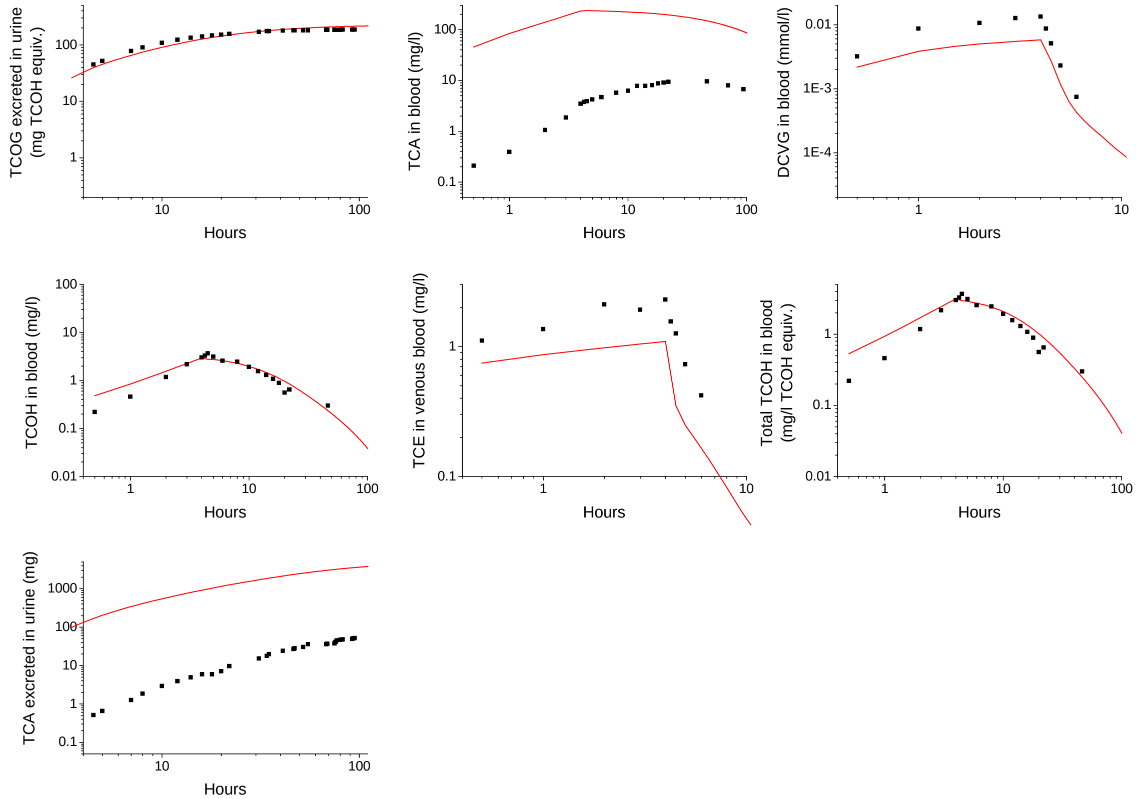
Fisher *et al.* 1998 Human #11 (sex=Female) – 53 ppm TCE 4 hour Inhalation



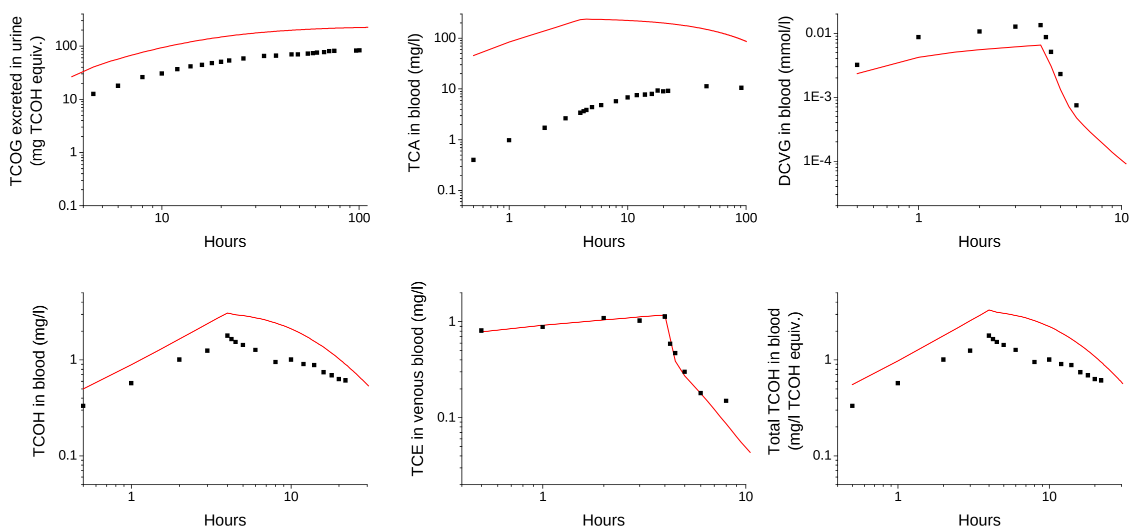
Fisher *et al.* 1998 Human #11 (sex=Female) – 97.7 ppm TCE 4 hour Inhalation



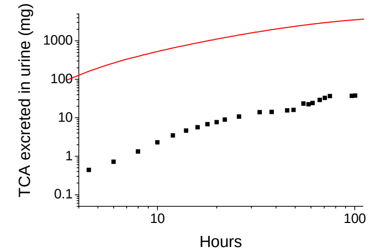
Fisher *et al.* 1998 Human #12 (sex=Female) – 102.5 ppm TCE 4 hour Inhalation



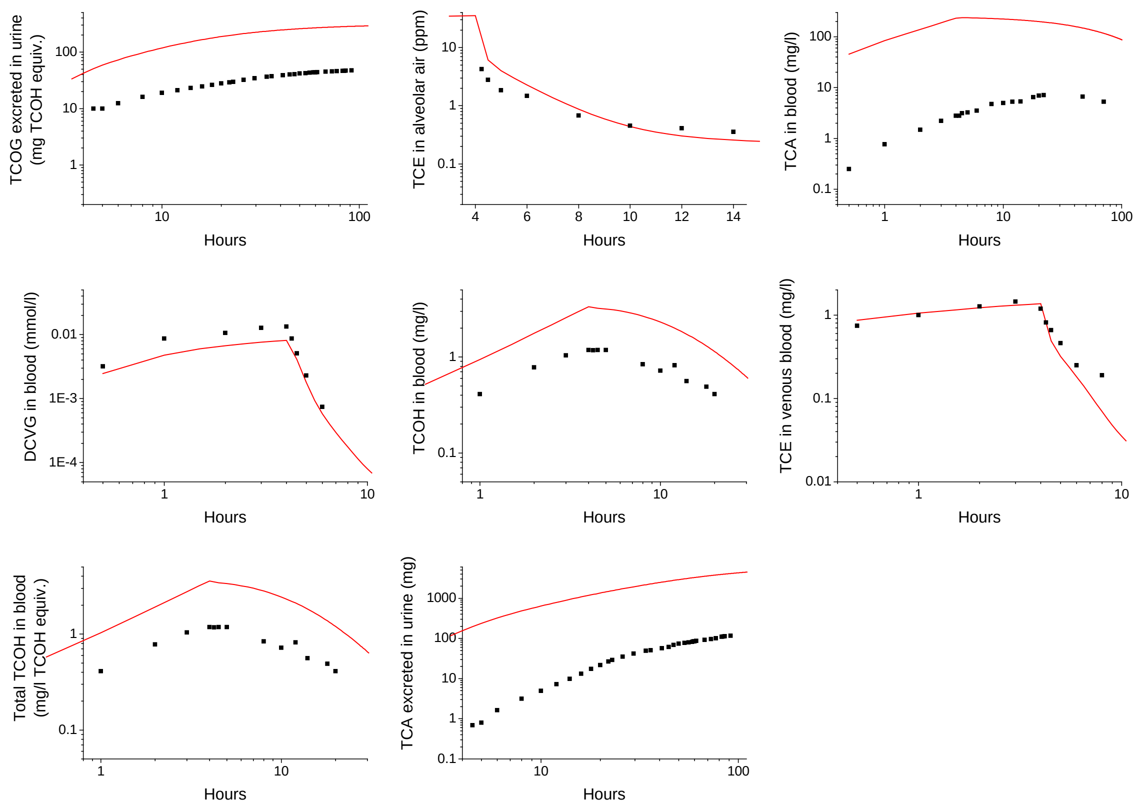
Fisher *et al.* 1998 Human #13 (sex=Female) – 102 ppm TCE 4 hour Inhalation



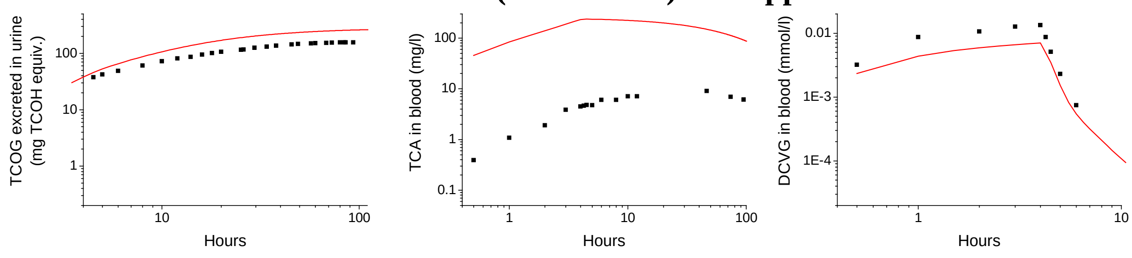
Fisher *et al.* 1998 Human #13 (sex=Female) – 102 ppm TCE 4 hour Inhalation



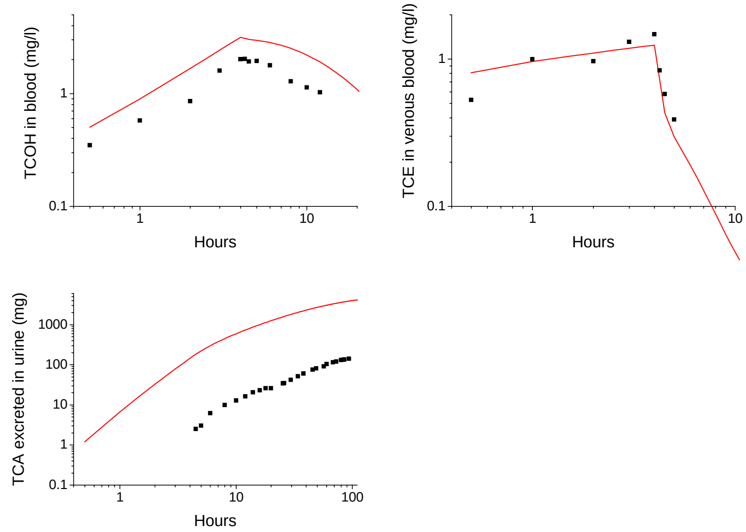
Fisher *et al.* 1998 Human #14 (sex=Female) – 102 ppm TCE 4 hour Inhalation



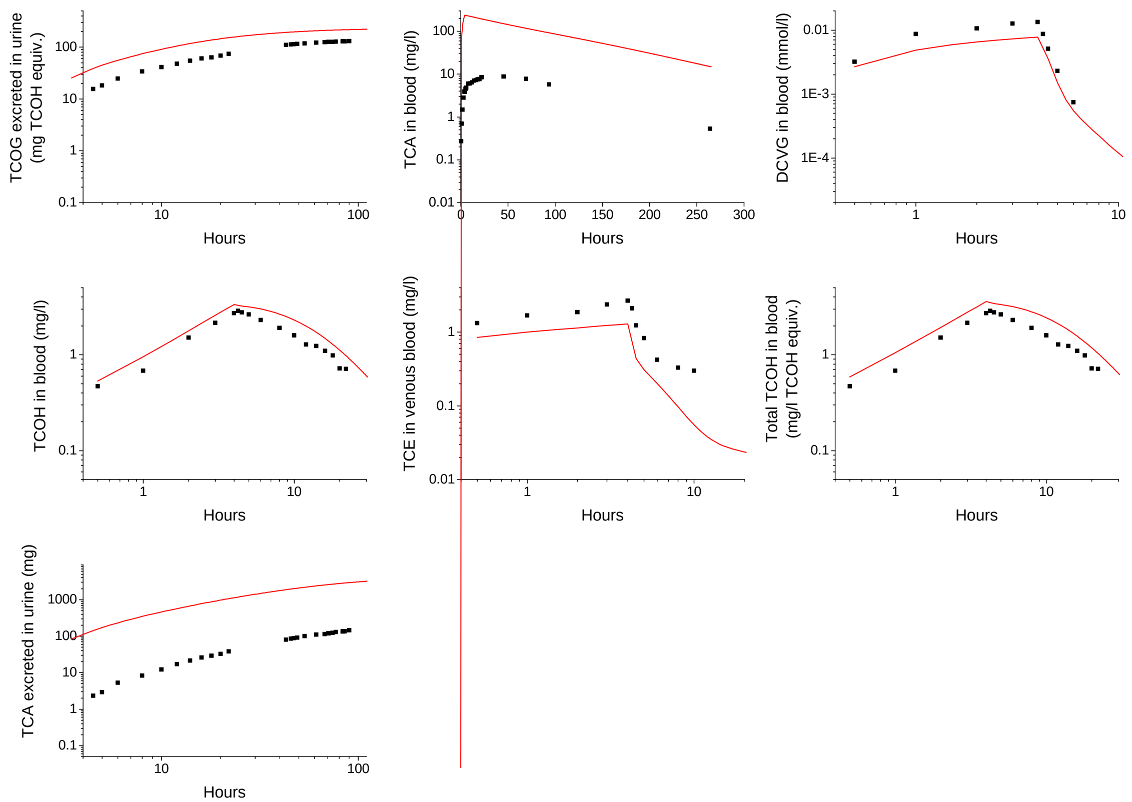
Fisher *et al.* 1998 Human #15 (sex=Female) – 101 ppm TCE 4 hour Inhalation



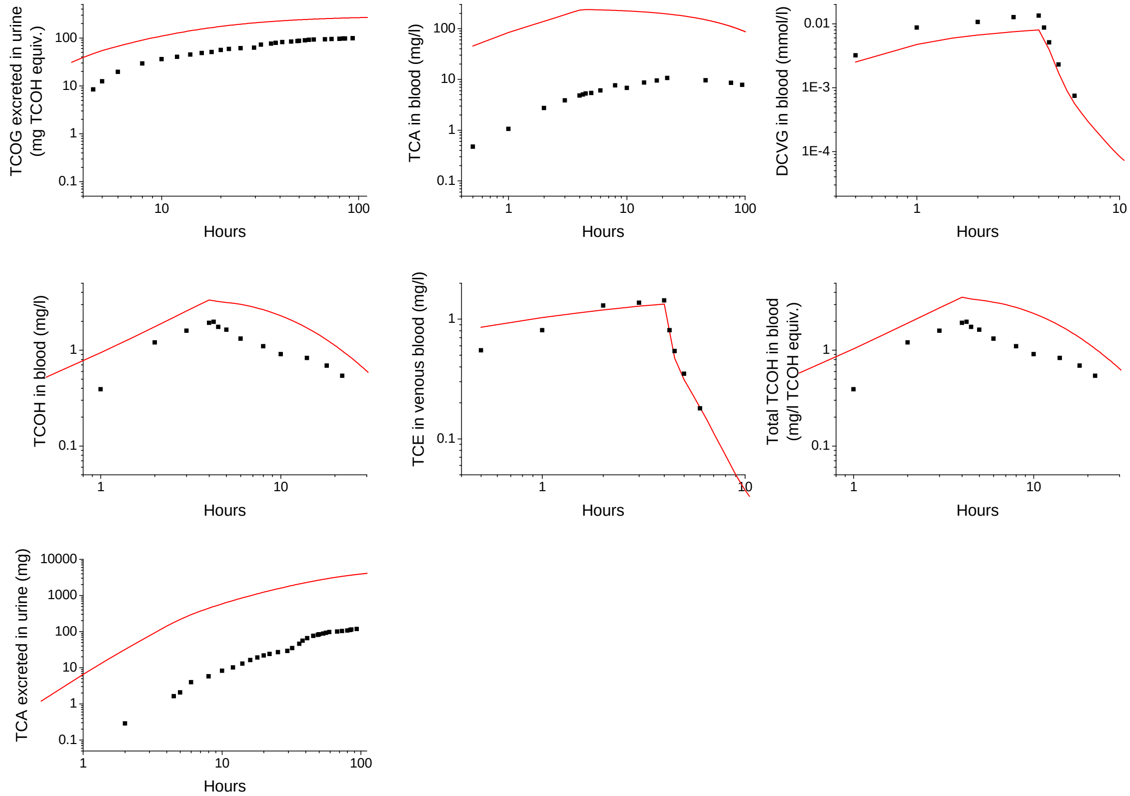
Fisher *et al.* 1998 Human #15 (sex=Female) – 101 ppm TCE 4 hour Inhalation



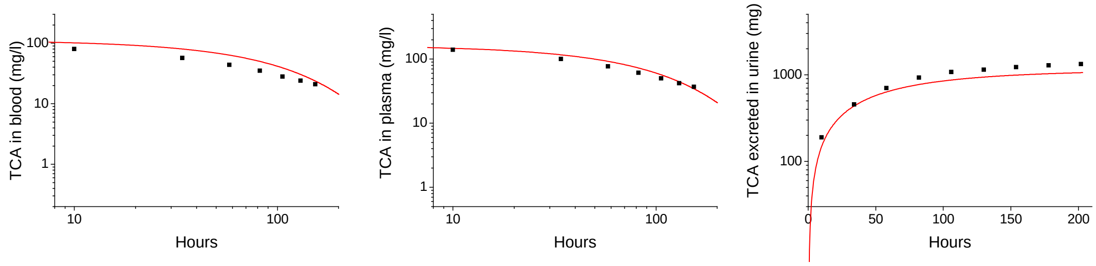
Fisher *et al.* 1998 Human #16 (sex=Female) – 103.3 ppm TCE 4 hour Inhalation



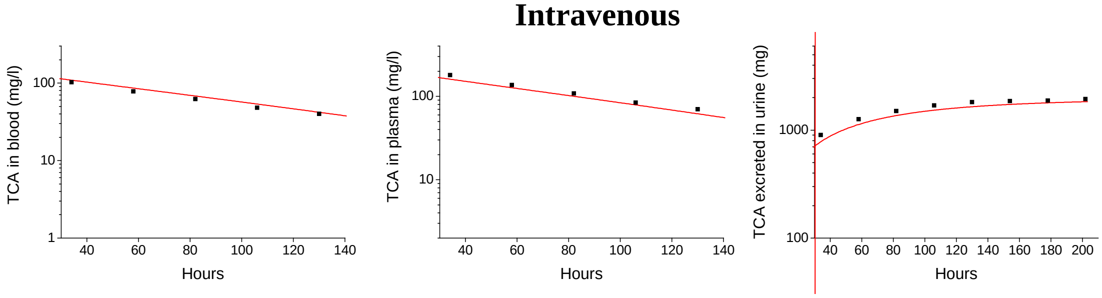
Fisher *et al.* 1998 Human #17 (sex=Female) – 102 ppm TCE 4 hour Inhalation



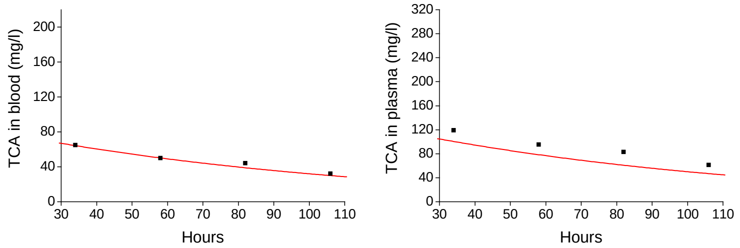
Paykoc and Powell 1945 Human #18 (sex=unknown) – 32.9 mg/kg TCA 1 hour Intravenous



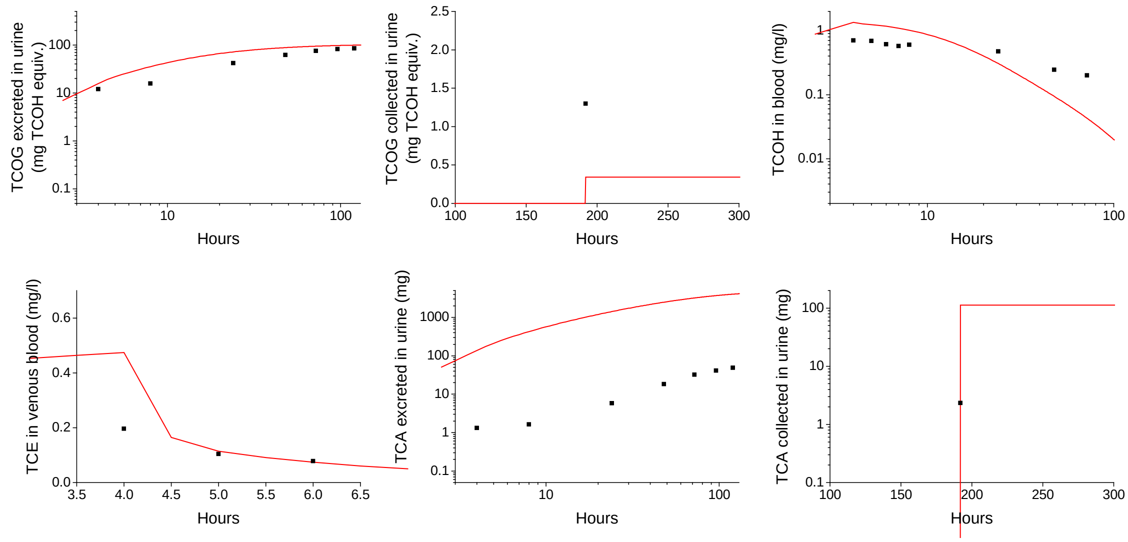
Paykoc and Powell 1945 Human #19 (sex=unknown) – 53.06 mg/kg TCA 1 hour Intravenous



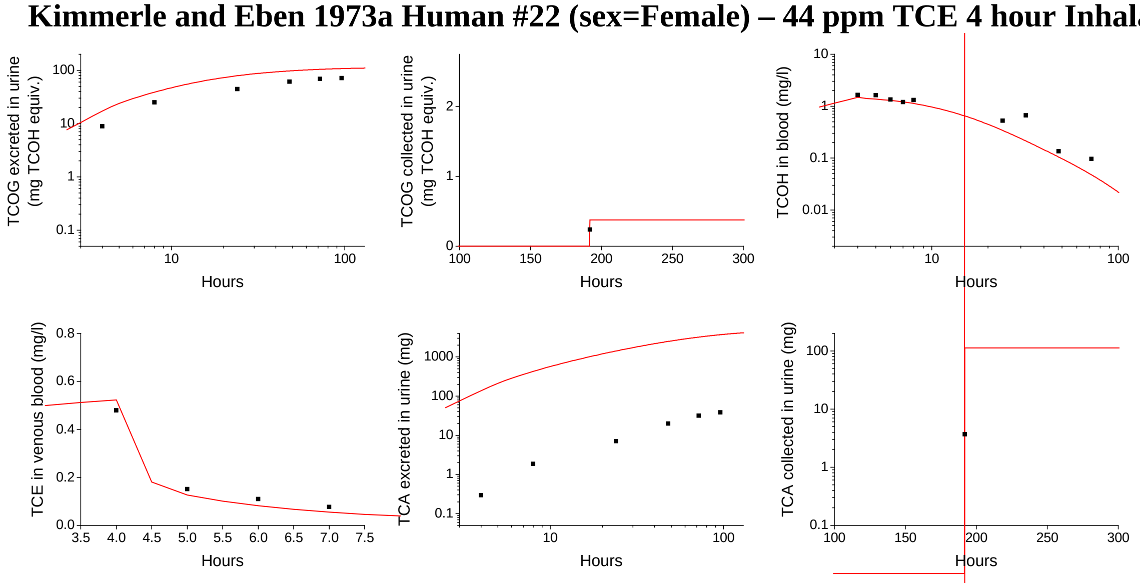
Paykoc and Powell 1945 Human #20 (sex=unknown) – 24.8 mg/kg TCA 1 hour Intravenous



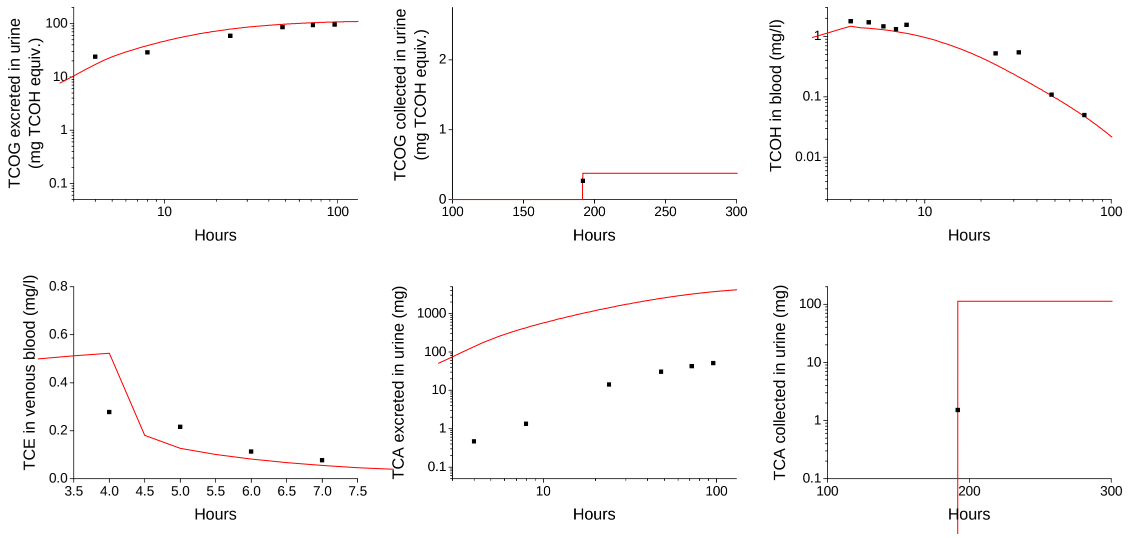
Kimmerle and Eben 1973a Human #21 (sex=Female) – 40 ppm TCE 4 hour Inhalation



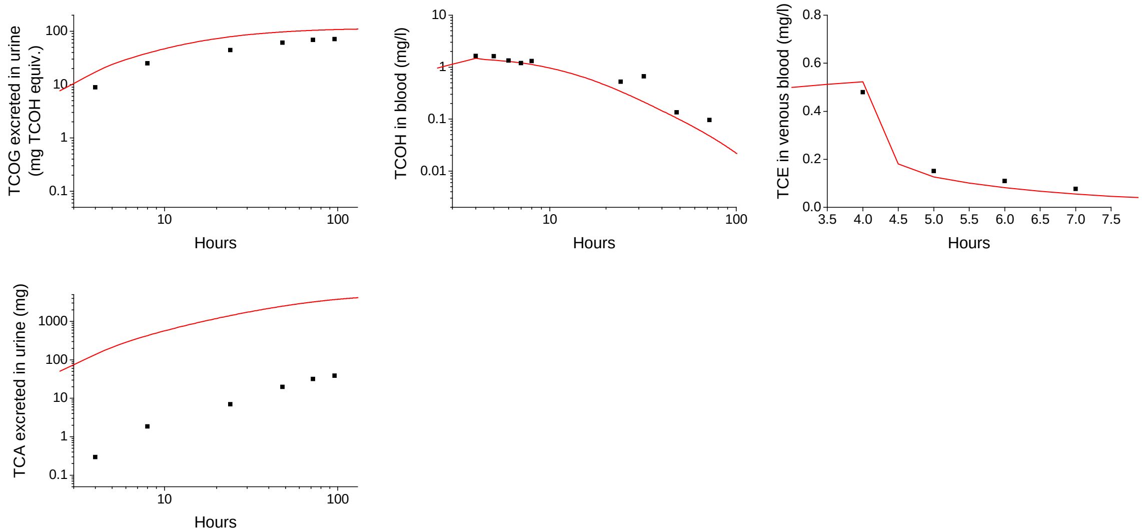
Kimmerle and Eben 1973a Human #22 (sex=Female) – 44 ppm TCE 4 hour Inhalation



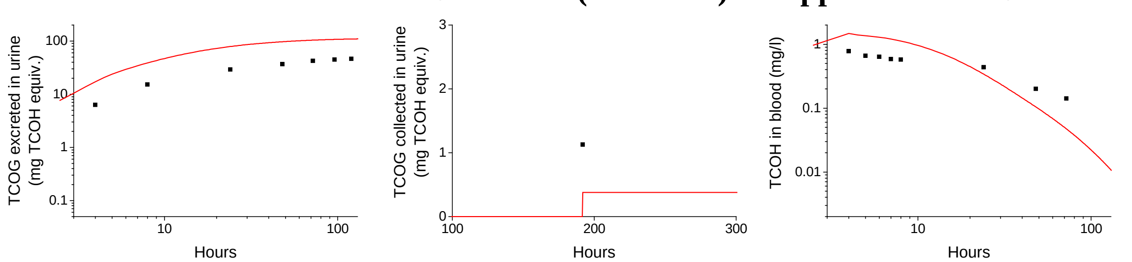
Kimmerle and Eben 1973a Human #23 (sex=Female) – 44 ppm TCE 4 hour Inhalation



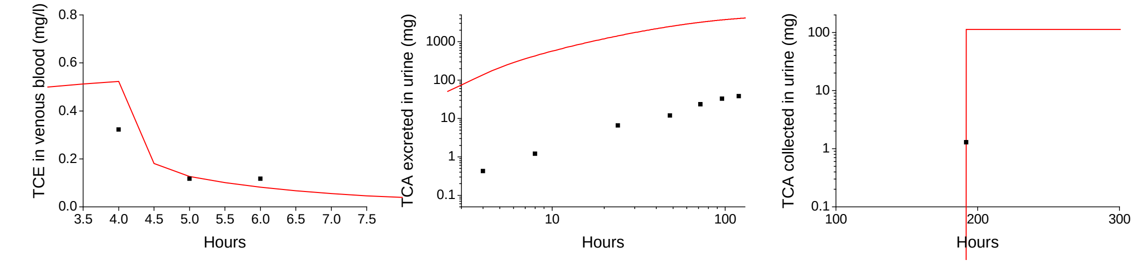
Kimmerle and Eben 1973a Human #24 (sex=Female) – 44 ppm TCE 4 hour Inhalation



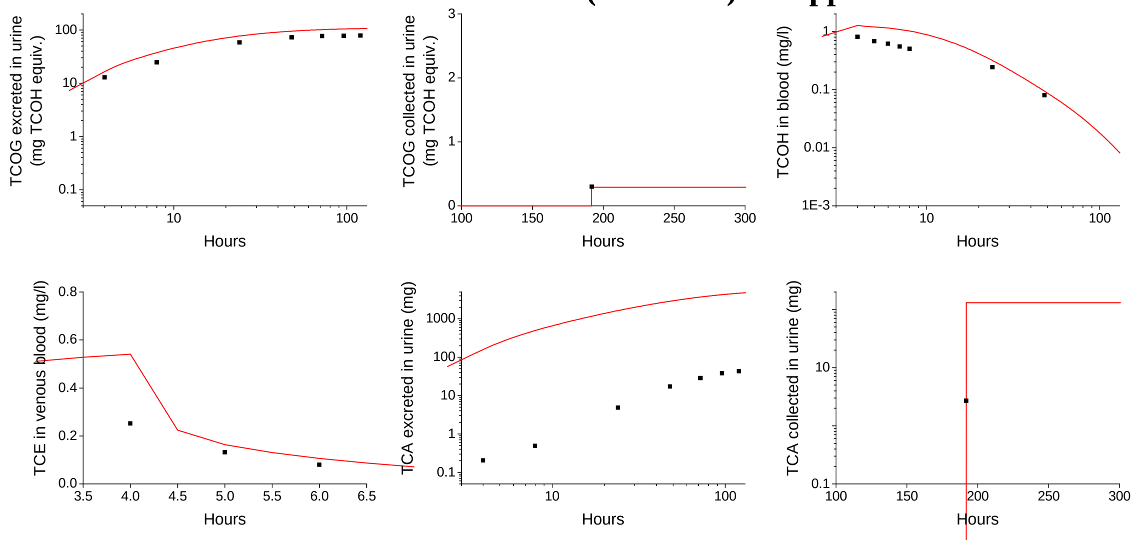
Kimmerle and Eben 1973a Human #25 (sex=Male) – 40 ppm TCE 4 hour Inhalation



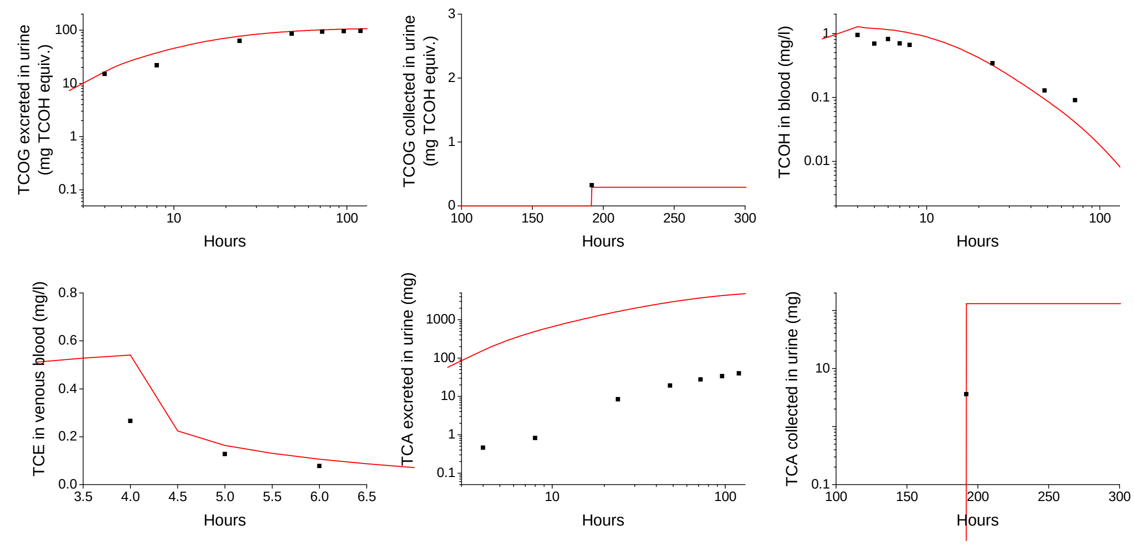
Kimmerle and Eben 1973a Human #25 (sex=Male) – 40 ppm TCE 4 hour Inhalation



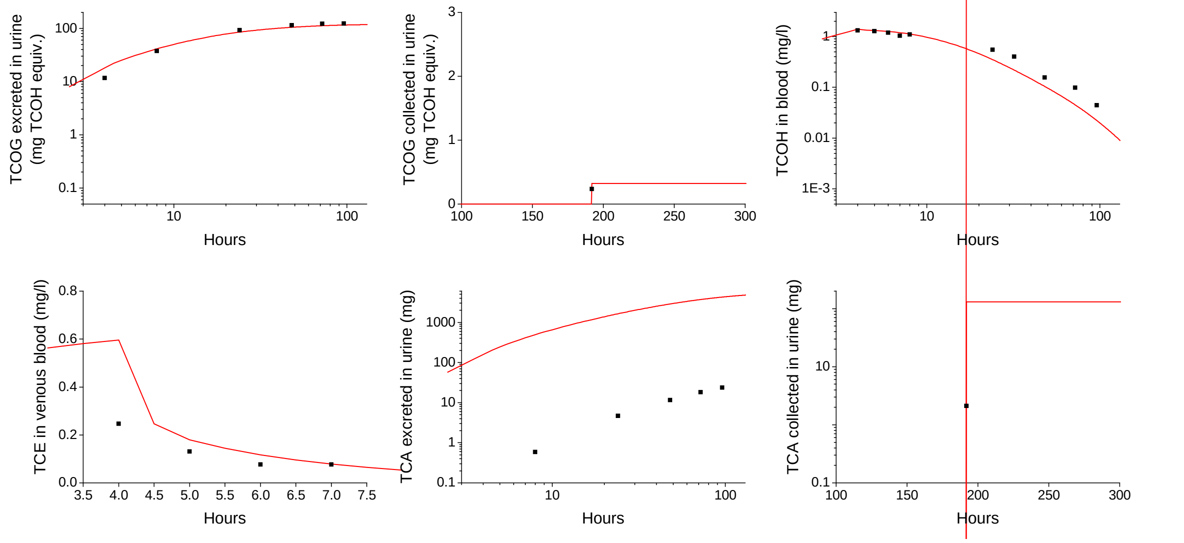
Kimmerle and Eben 1973a Human #26 (sex=Male) – 40 ppm TCE 4 hour Inhalation



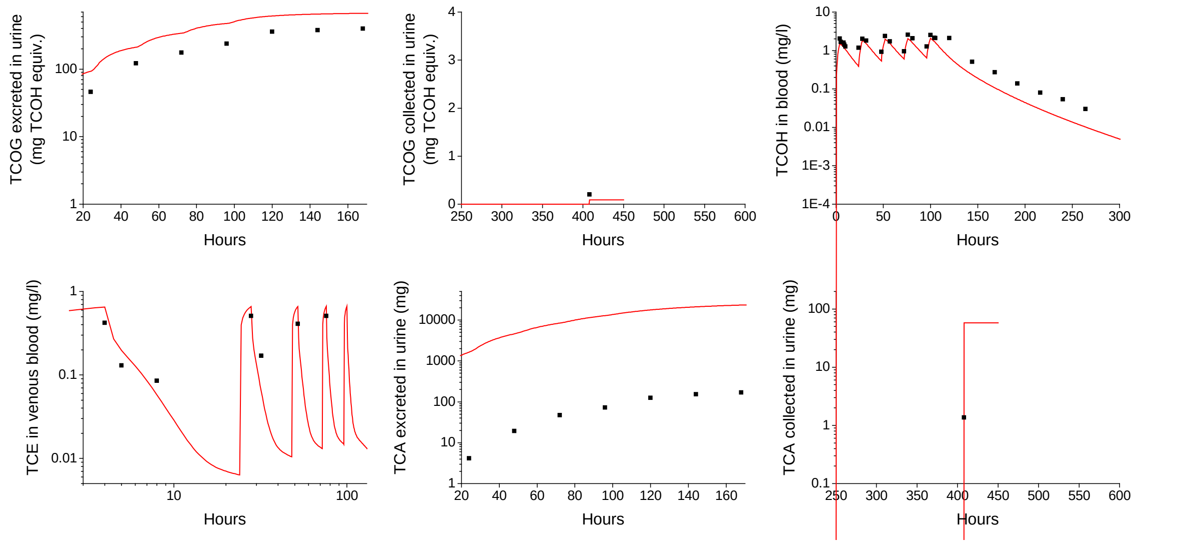
Kimmerle and Eben 1973a Human #27 (sex=Male) – 40 ppm TCE 4 hour Inhalation



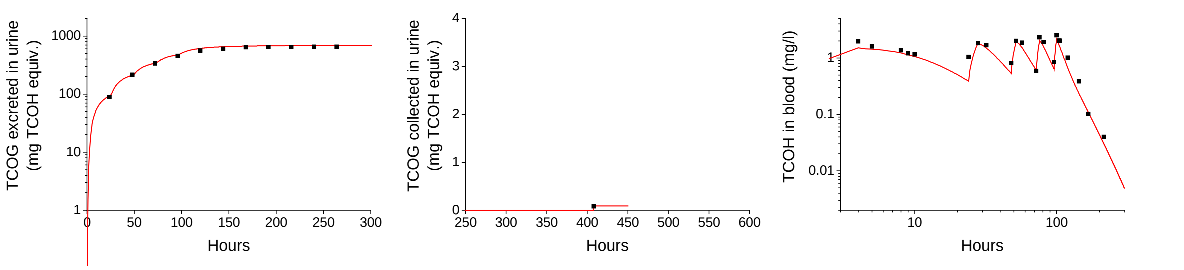
Kimmerle and Eben 1973a Human #28 (sex=Male) – 44 ppm TCE 4 hour Inhalation



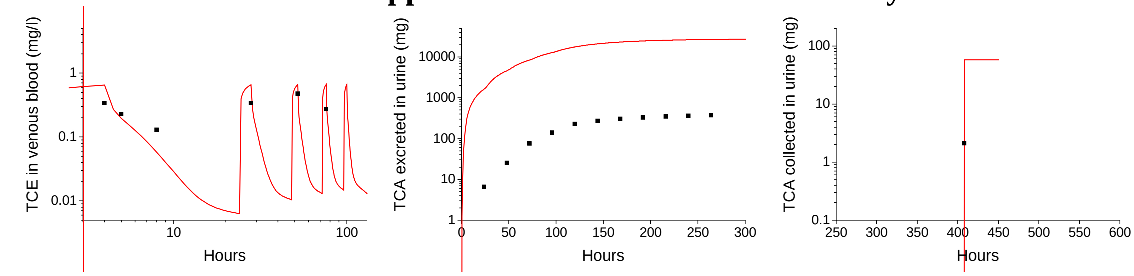
Kimmerle and Eben 1973a Human #29 (sex=unknown) – 48 ppm TCE 4 hour Inhalation for 5 days



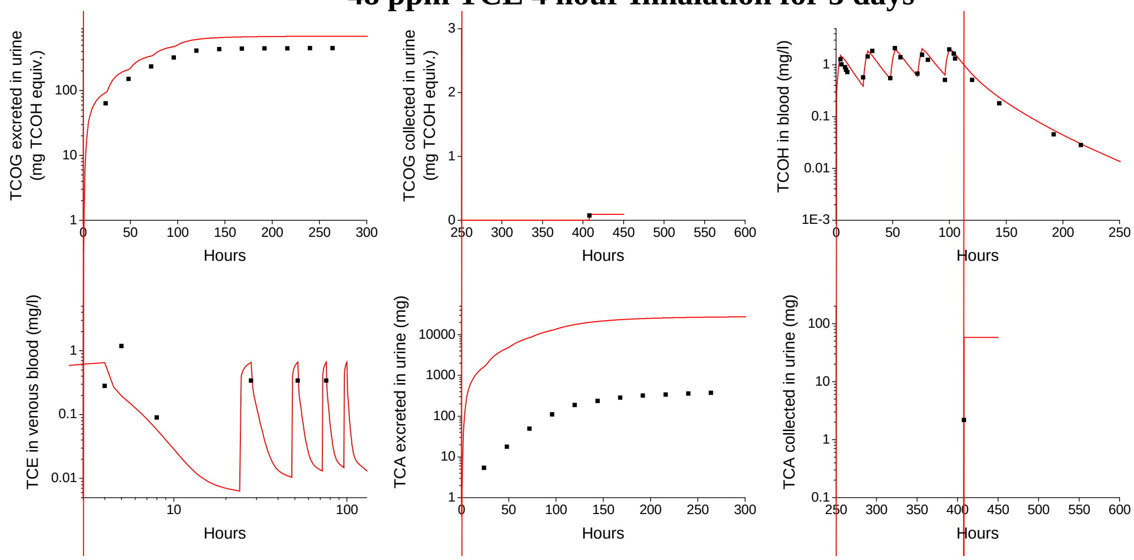
Kimmerle and Eben 1973a Human #30 (sex=unknown) – 48 ppm TCE 4 hour Inhalation for 5 days



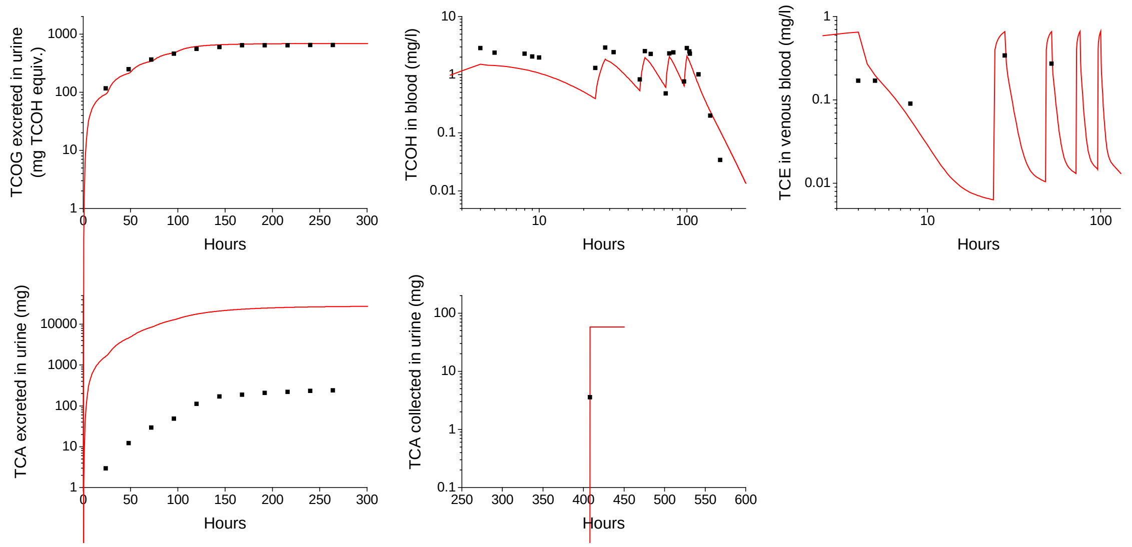
Kimmerle and Eben 1973a Human #30 (sex=unknown) – 48 ppm TCE 4 hour Inhalation for 5 days



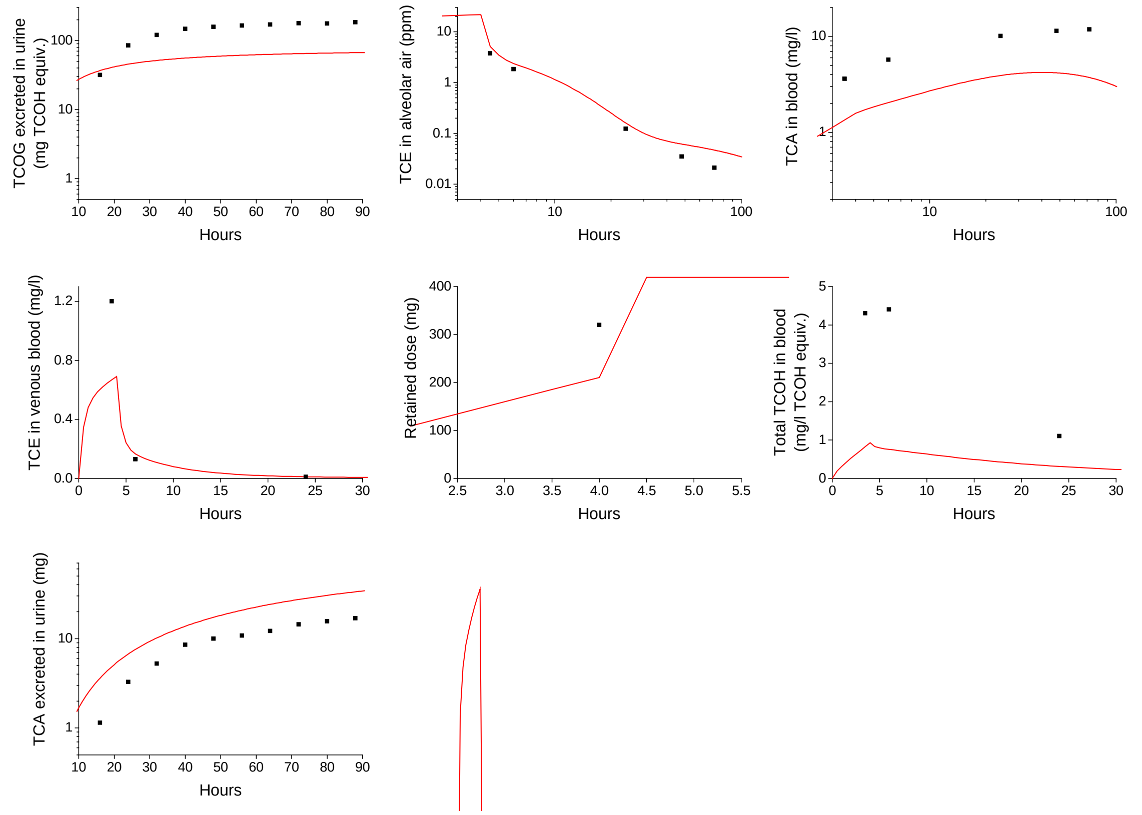
Kimmerle and Eben 1973a Human #31 (sex=unknown) – 48 ppm TCE 4 hour Inhalation for 5 days



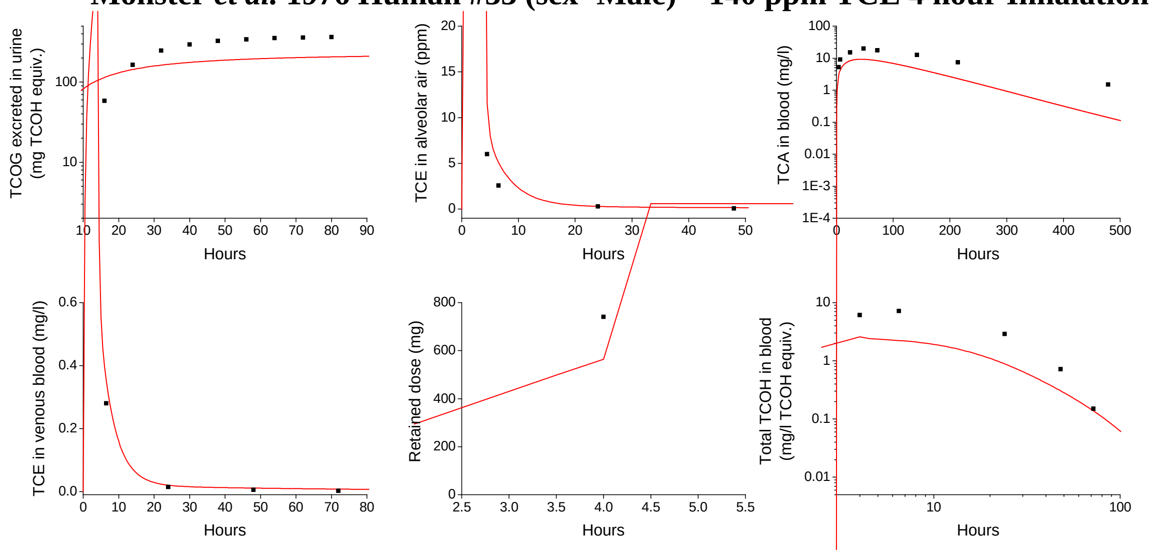
Kimmerle and Eben 1973a Human #32 (sex=unknown) – 48 ppm TCE 4 hour Inhalation for 5 days



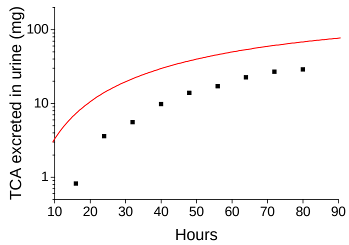
Monster *et al.* 1976 Human #33 (sex=Male) – 65 ppm TCE 4 hour Inhalation



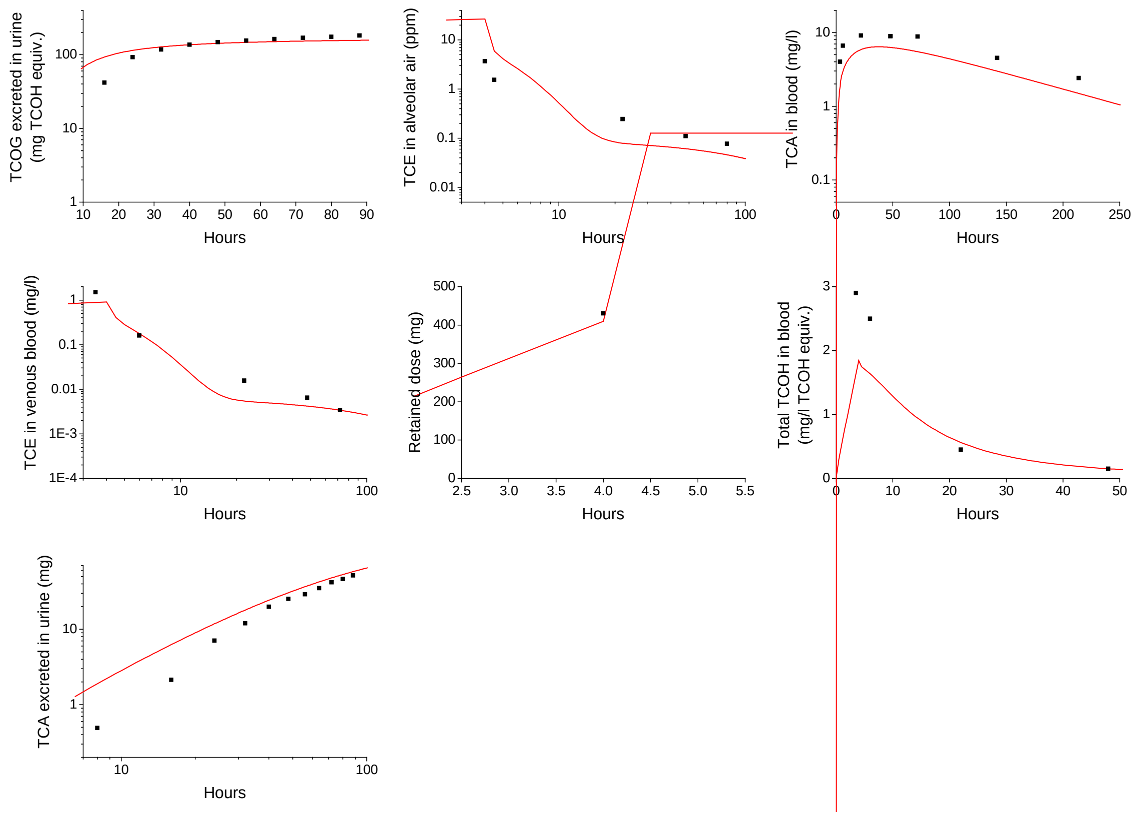
Monster *et al.* 1976 Human #33 (sex=Male) – 140 ppm TCE 4 hour Inhalation



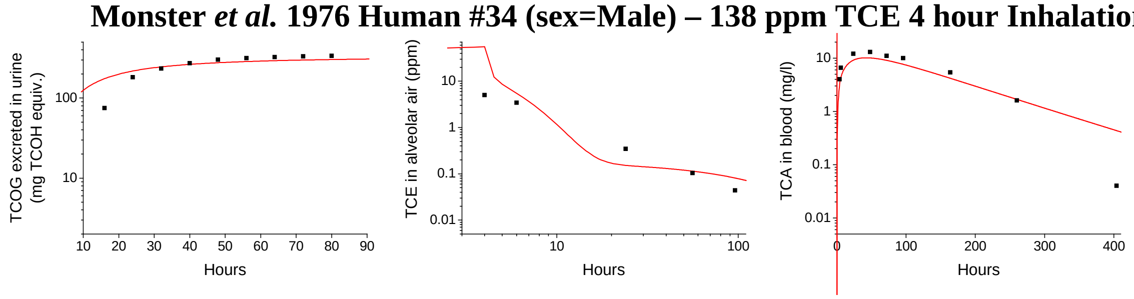
Monster *et al.* 1976 Human #33 (sex=Male) – 140 ppm TCE 4 hour Inhalation



Monster *et al.* 1976 Human #34 (sex=Male) – 68 ppm TCE 4 hour Inhalation

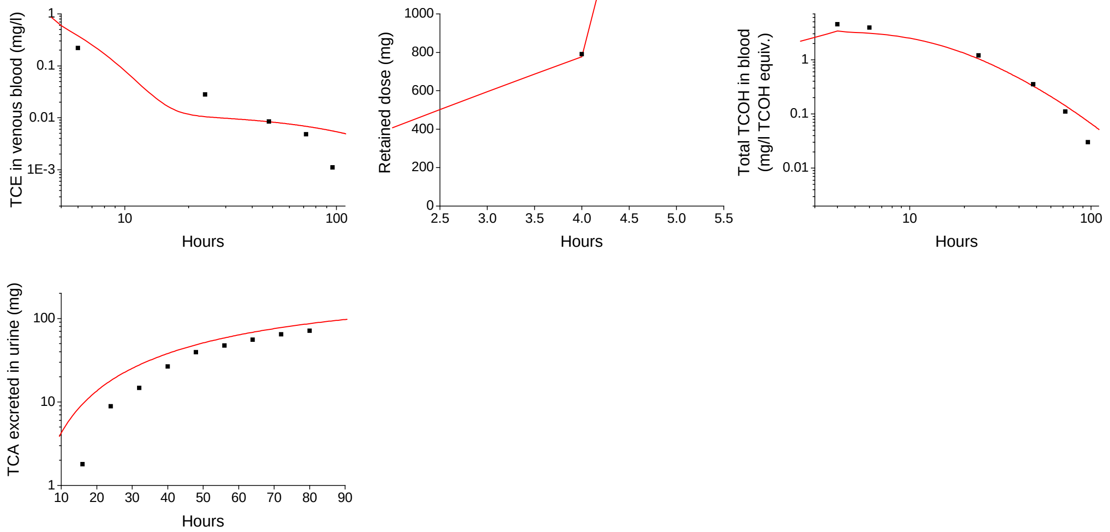


Monster *et al.* 1976 Human #34 (sex=Male) – 138 ppm TCE 4 hour Inhalation

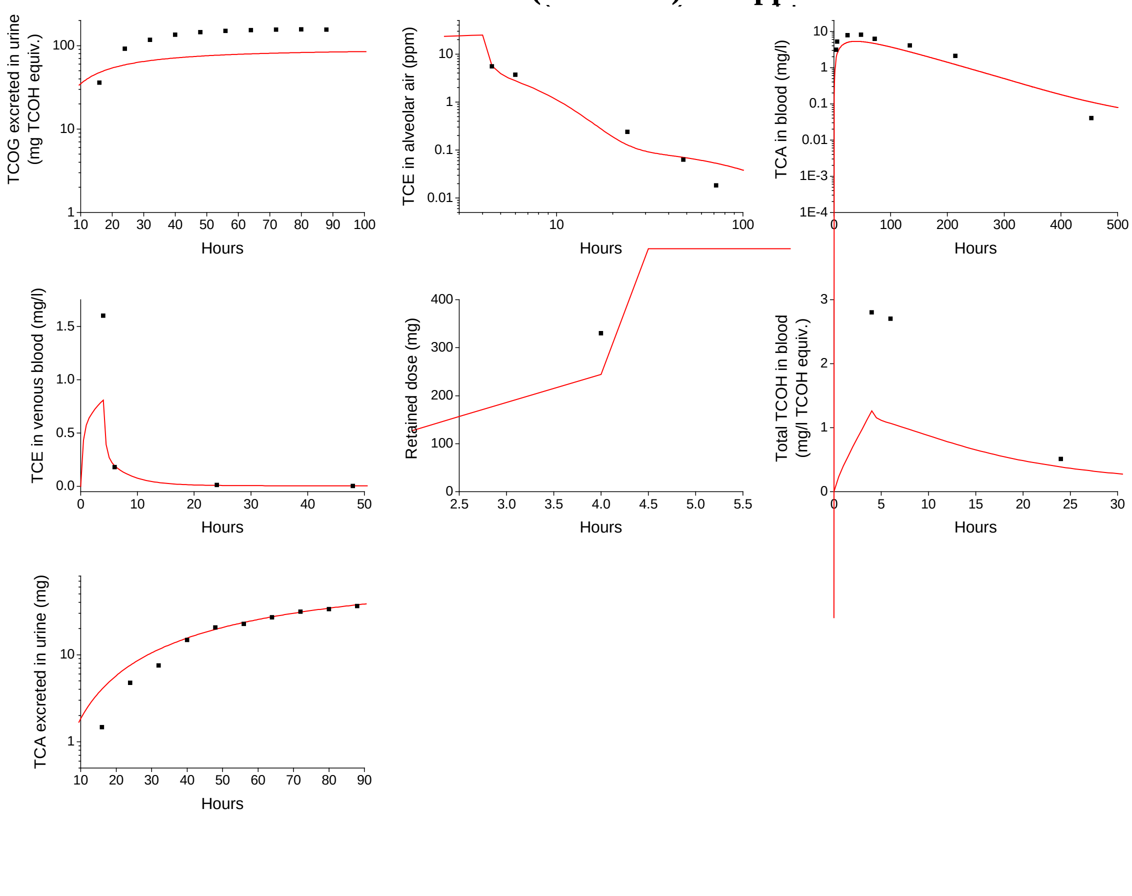


Distribution A: Approved for public release; distribution unlimited (PA Case No 88ABW-2017-XXXX, Date)

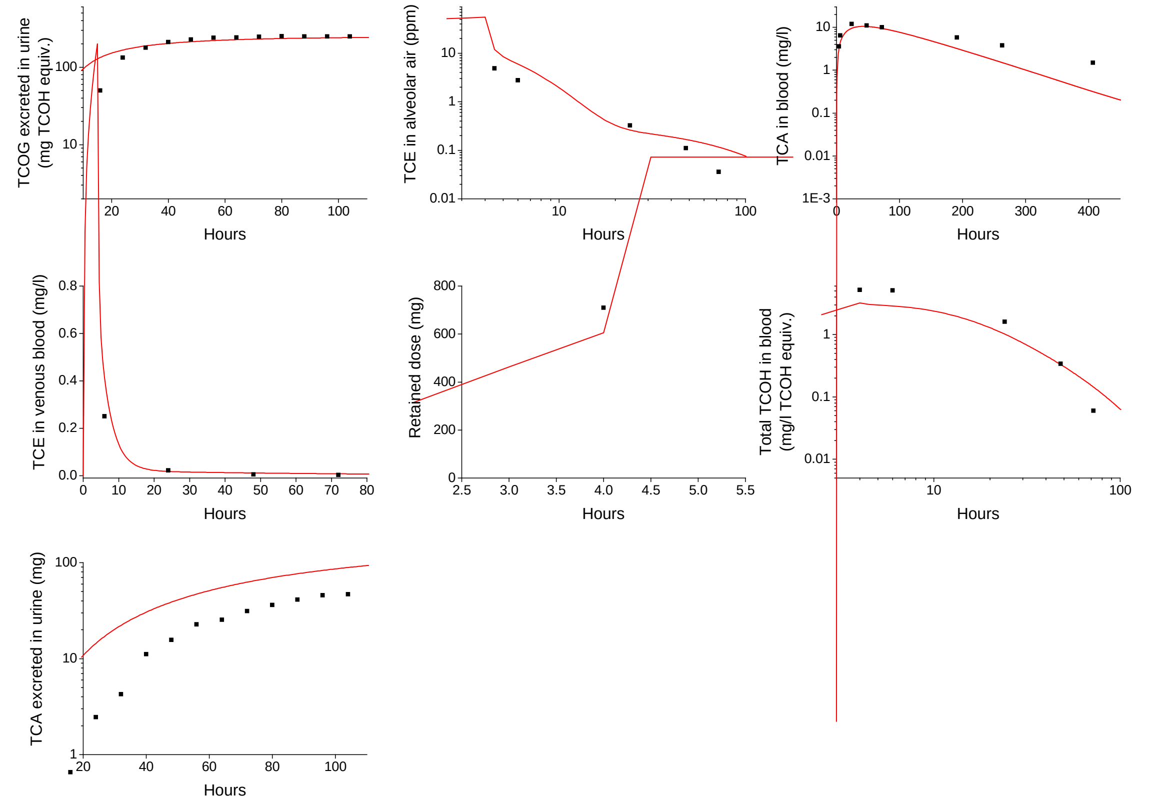
Monster *et al.* 1976 Human #34 (sex=Male) – 138 ppm TCE 4 hour Inhalation



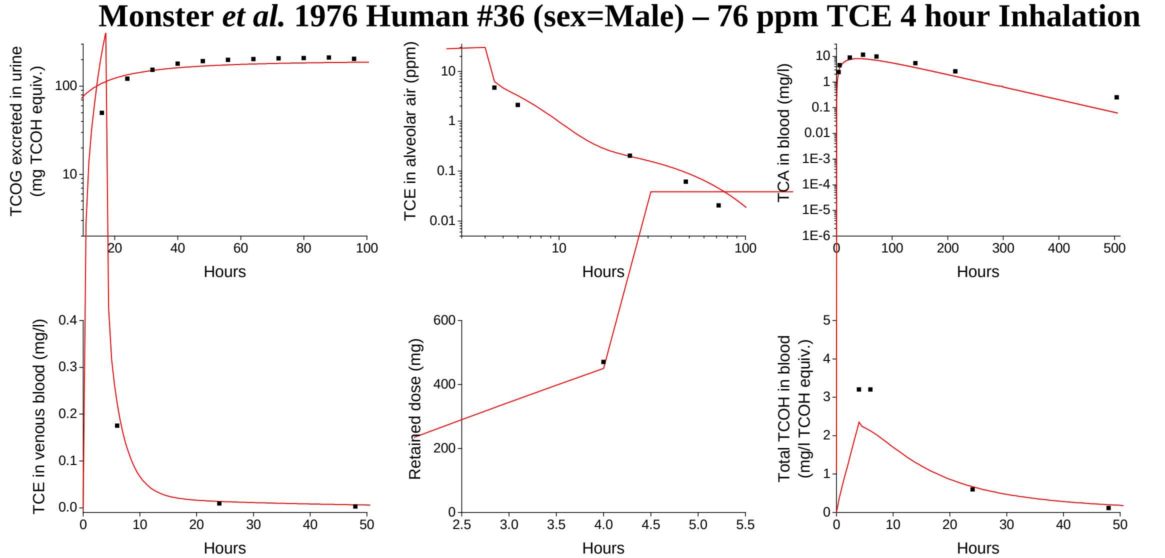
Monster *et al.* 1976 Human #35 (sex=Male) – 70 ppm TCE 4 hour Inhalation



Monster *et al.* 1976 Human #35 (sex=Male) – 142 ppm TCE 4 hour Inhalation

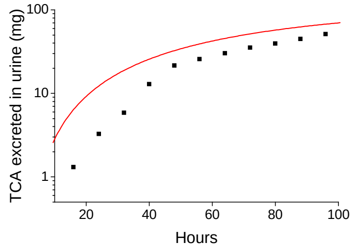


Monster *et al.* 1976 Human #36 (sex=Male) – 76 ppm TCE 4 hour Inhalation

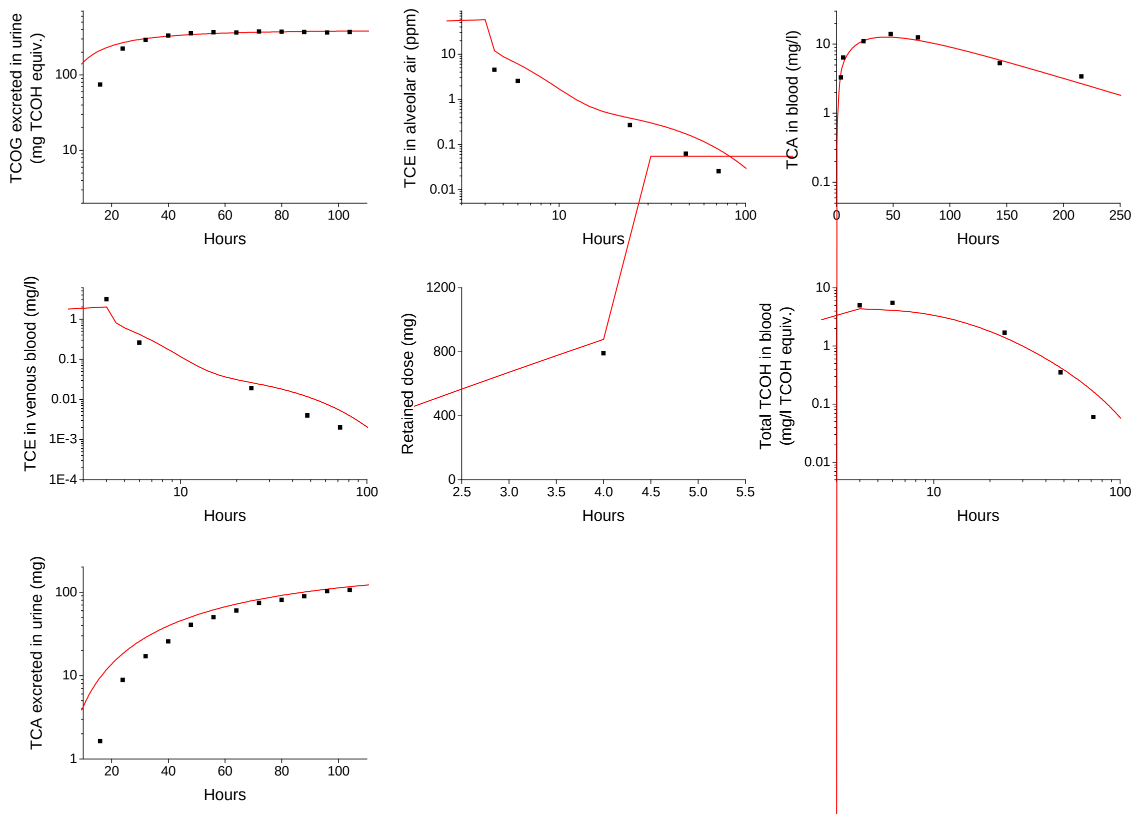


Distribution A: Approved for public release; distribution unlimited (PA Case No 88ABW-2017-XXXX, Date)

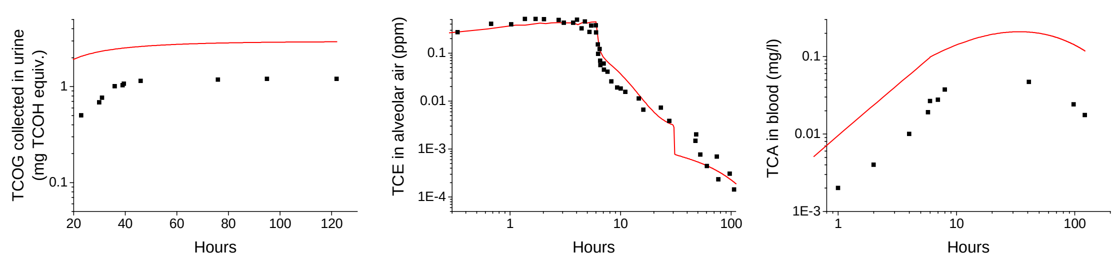
Monster *et al.* 1976 Human #36 (sex=Male) – 76 ppm TCE 4 hour Inhalation



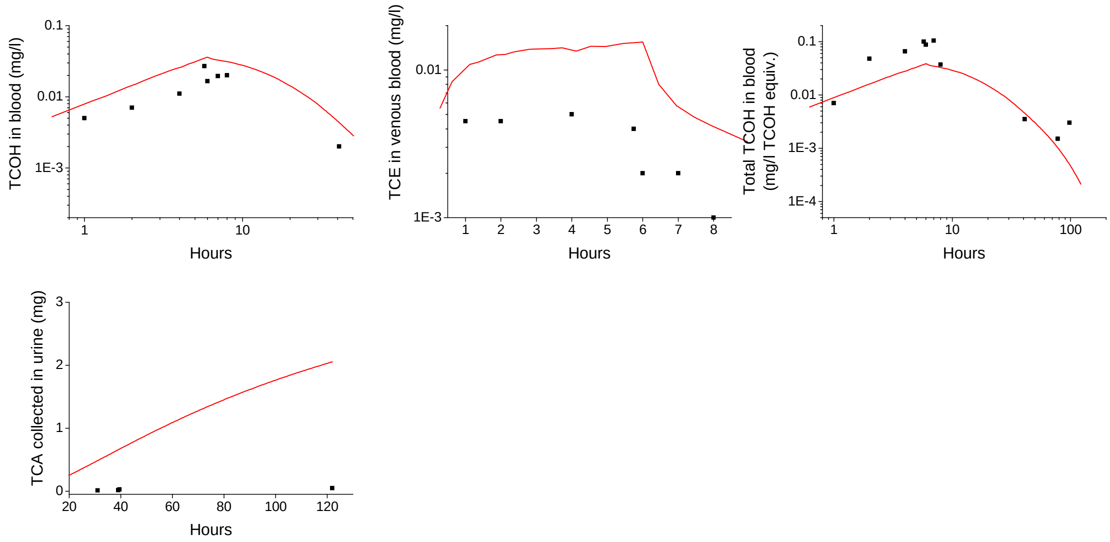
Monster *et al.* 1976 Human #36 (sex=Male) – 140 ppm TCE 4 hour Inhalation



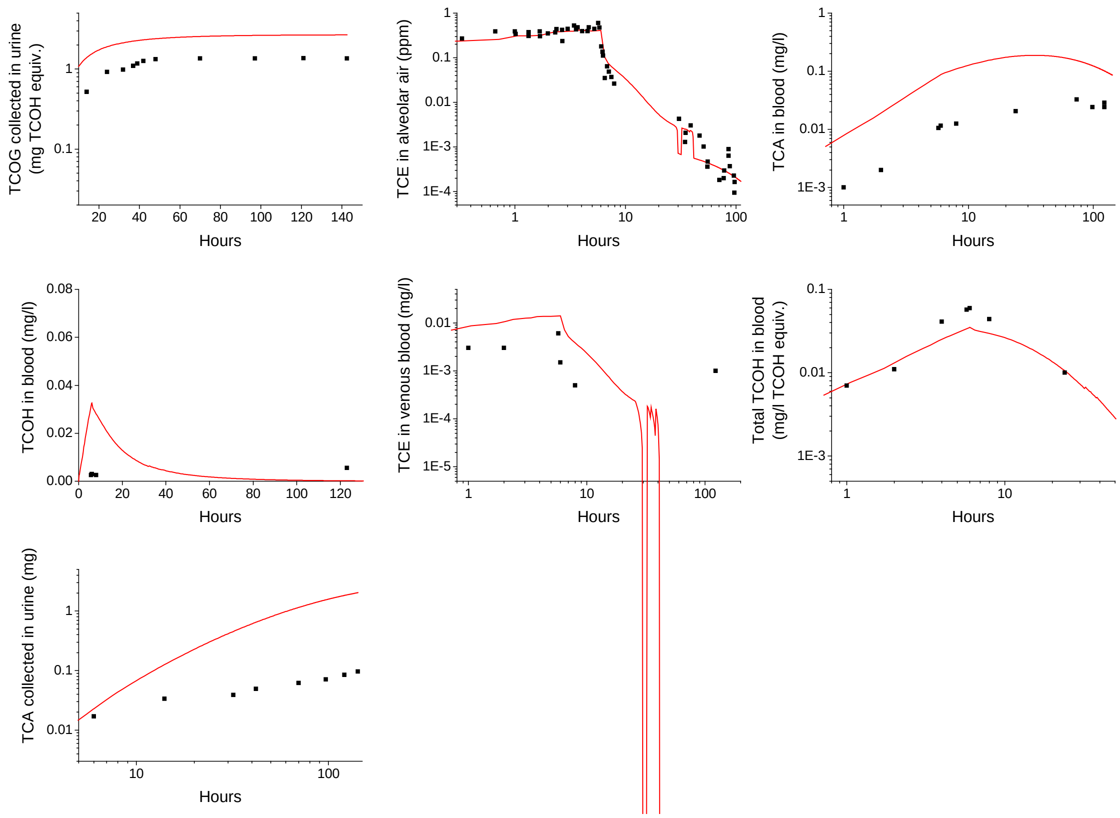
Chiu *et al.* 2007 Human #37 (sex=Male) – 1 ppm TCE 6 hour Inhalation



Chiu *et al.* 2007 Human #37 (sex=Male) – 1 ppm TCE 6 hour Inhalation

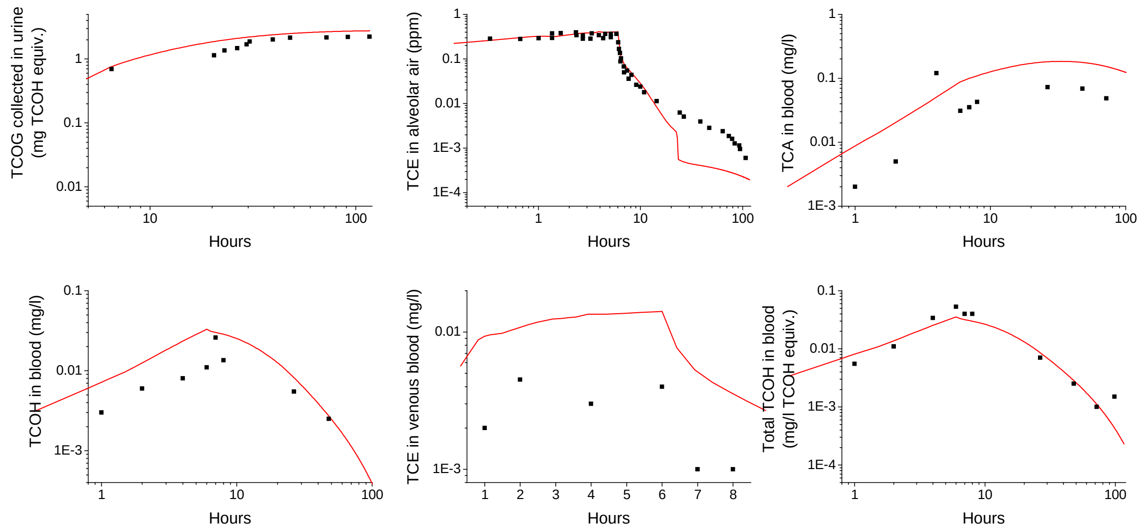


Chiu *et al.* 2007 Human #37 (sex=Male) – 1 ppm TCE 6 hour Inhalation

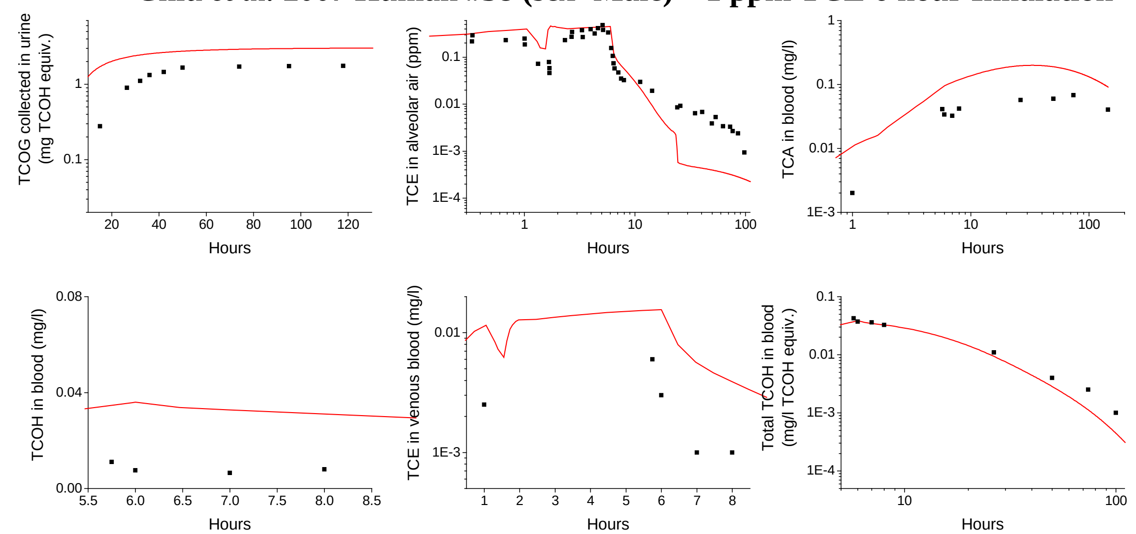


Distribution A: Approved for public release; distribution unlimited (PA Case No 88ABW-2017-XXXX, Date)

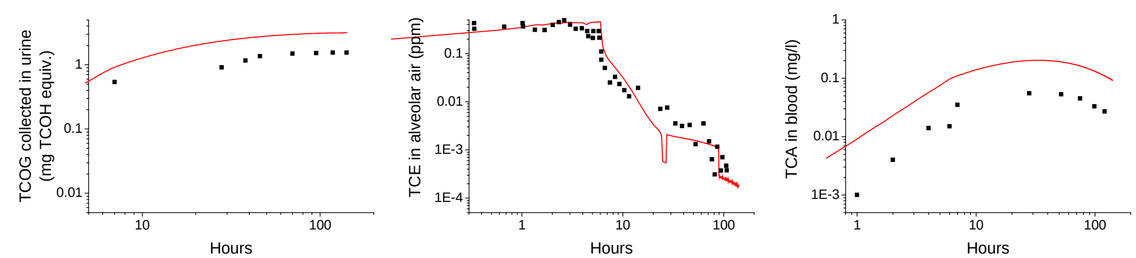
Chiu *et al.* 2007 Human #38 (sex=Male) – 1 ppm TCE 6 hour Inhalation



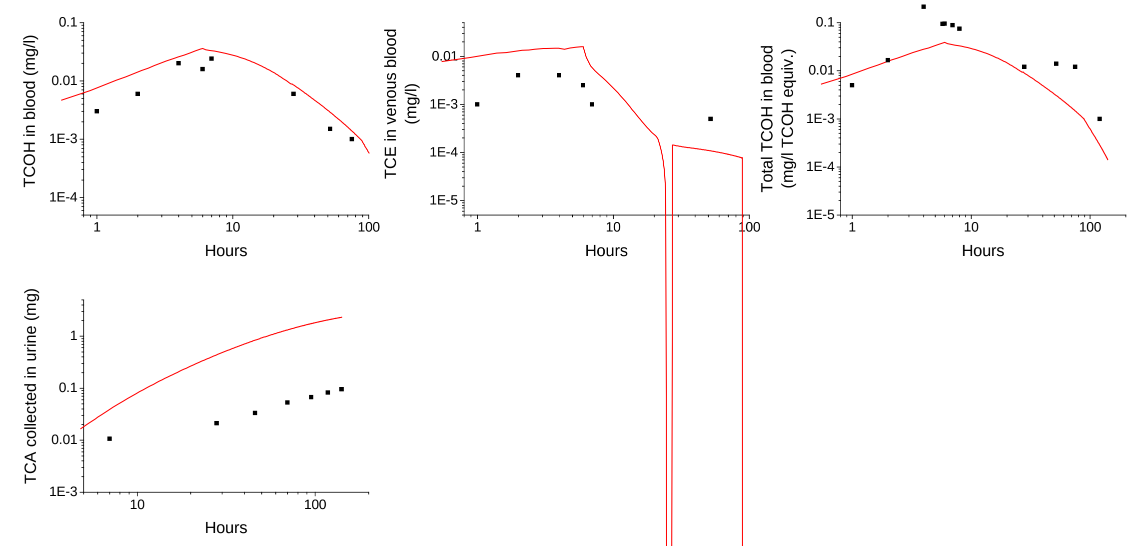
Chiu *et al.* 2007 Human #38 (sex=Male) – 1 ppm TCE 6 hour Inhalation



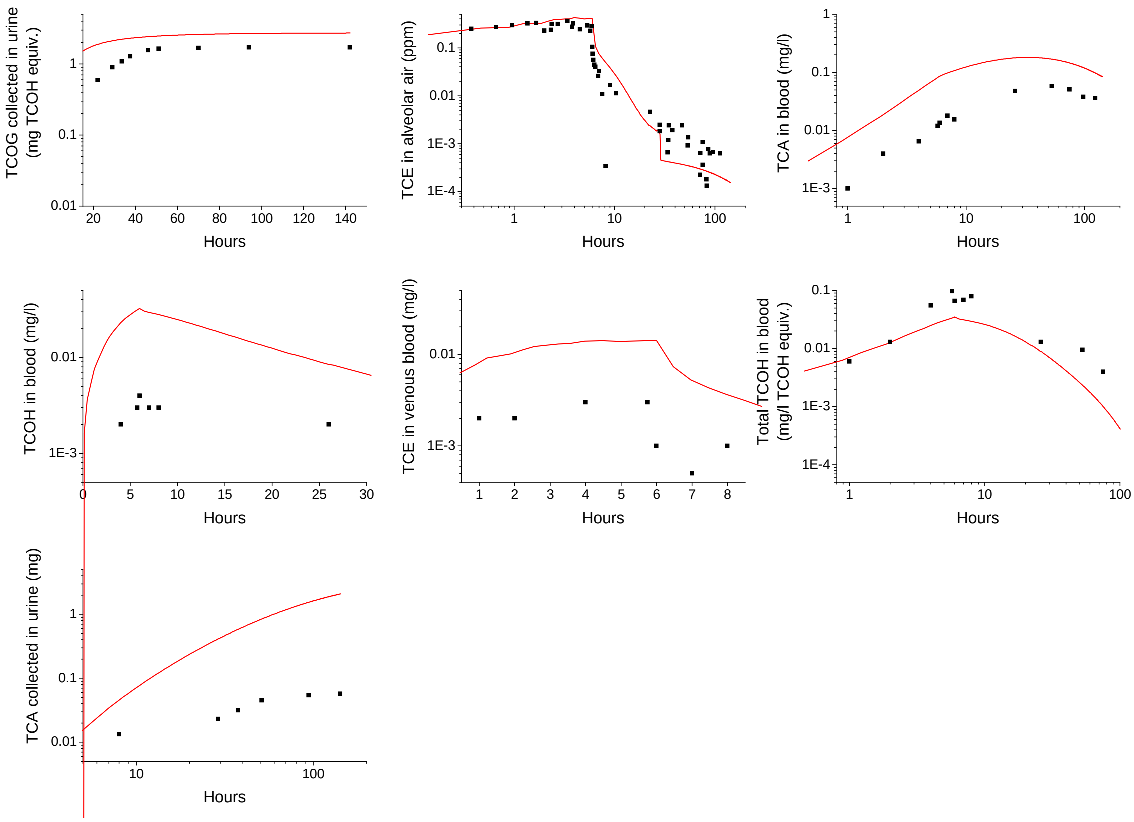
Chiu *et al.* 2007 Human #39 (sex=Male) – 1 ppm TCE 6 hour Inhalation



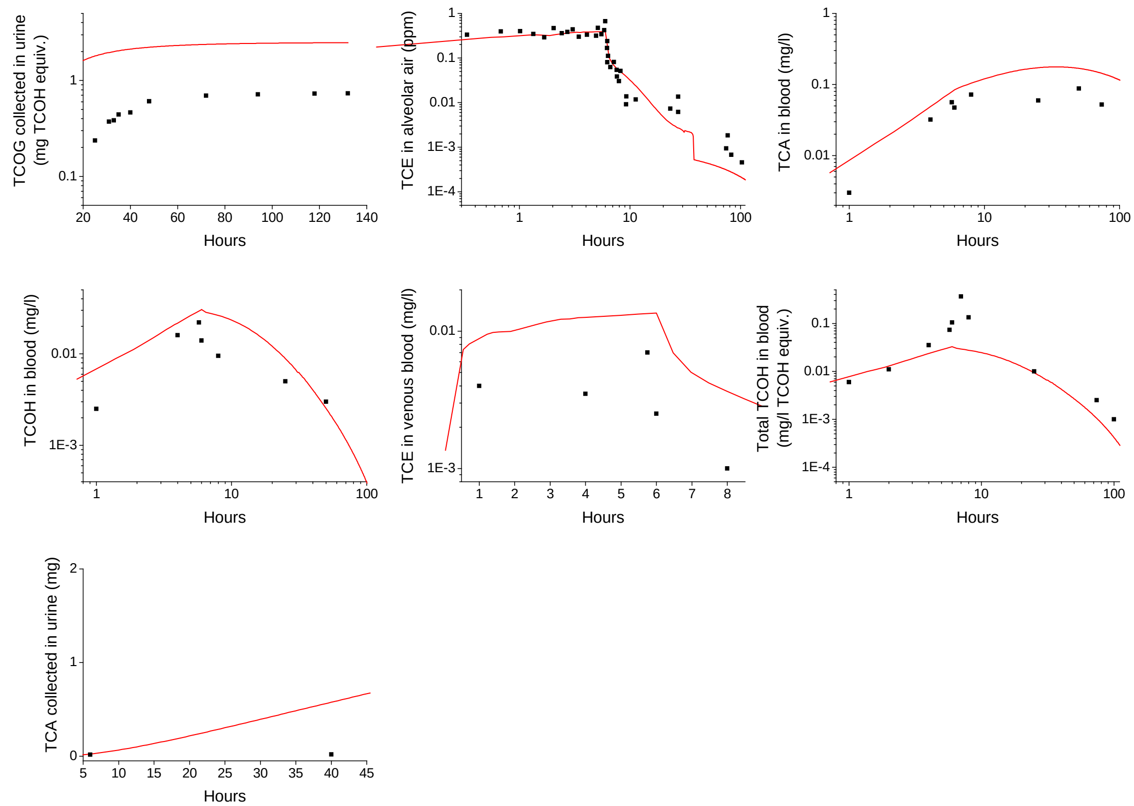
Chiu *et al.* 2007 Human #39 (sex=Male) – 1 ppm TCE 6 hour Inhalation



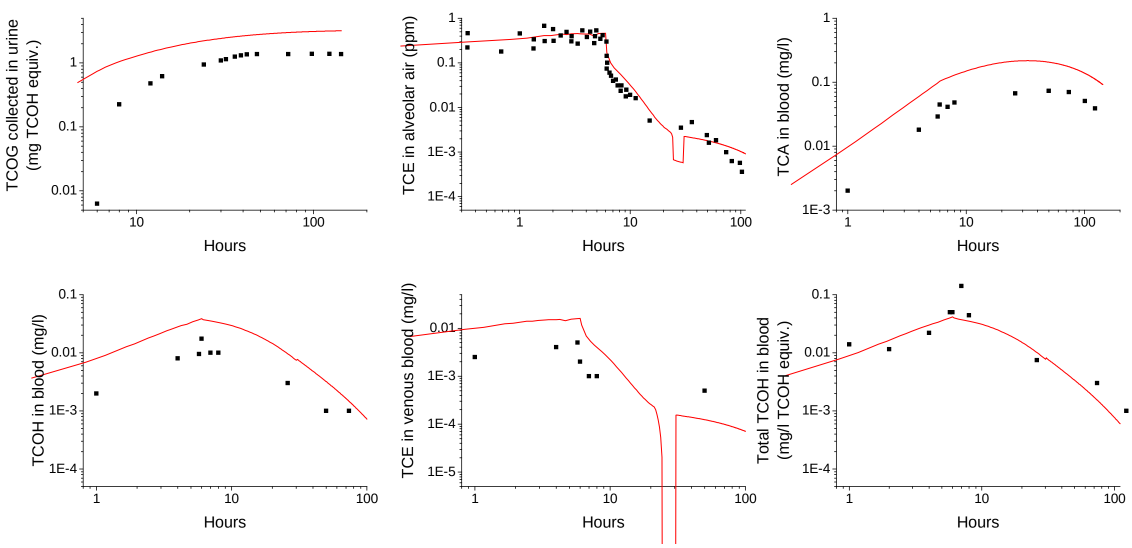
Chiu *et al.* 2007 Human #39 (sex=Male) – 1 ppm TCE 6 hour Inhalation



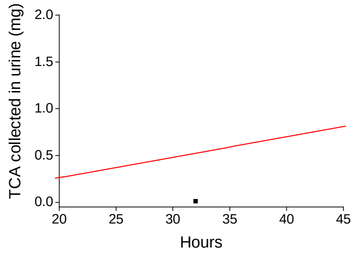
Chiu *et al.* 2007 Human #40 (sex=Male) – 1 ppm TCE 6 hour Inhalation



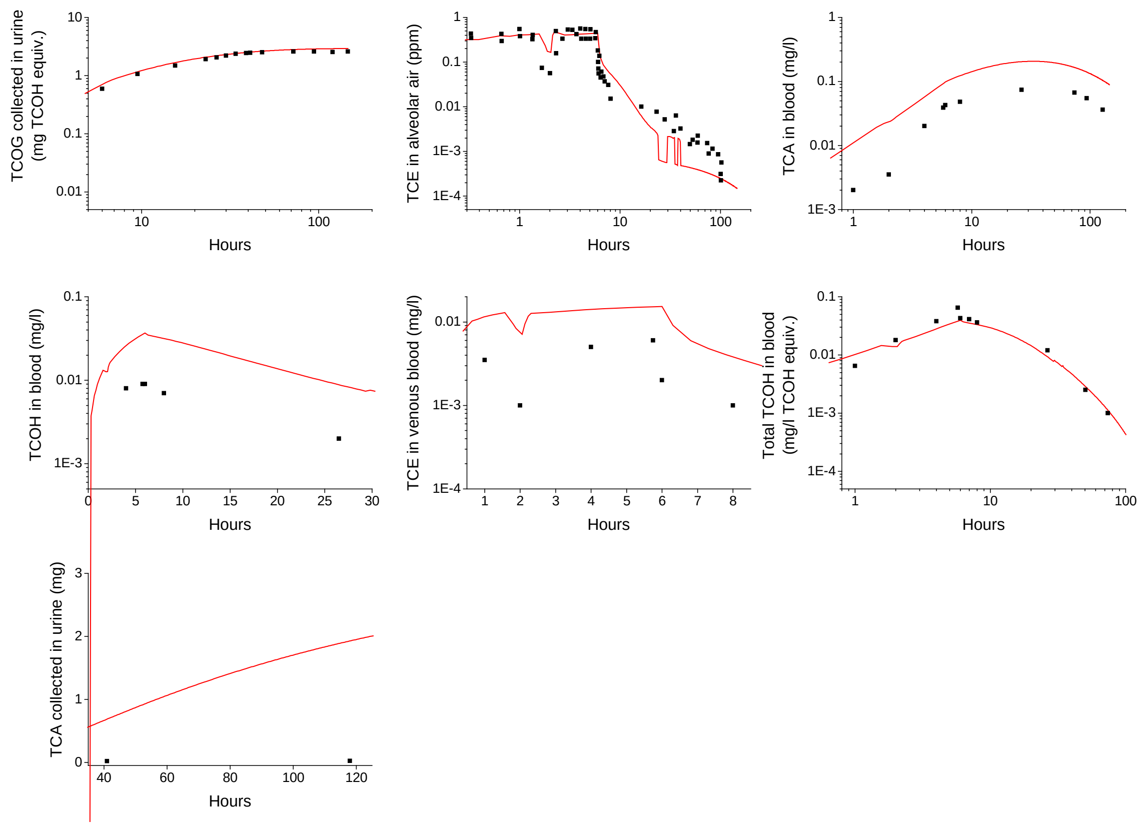
Chiu *et al.* 2007 Human #41 (sex=Male) – 1 ppm TCE 6 hour Inhalation



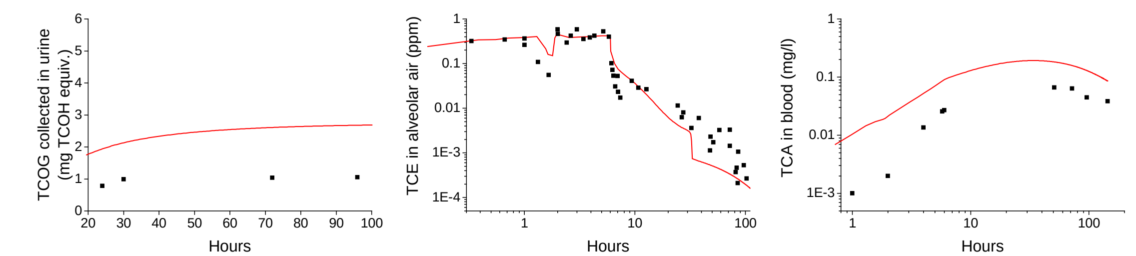
Chiu *et al.* 2007 Human #41 (sex=Male) – 1 ppm TCE 6 hour Inhalation



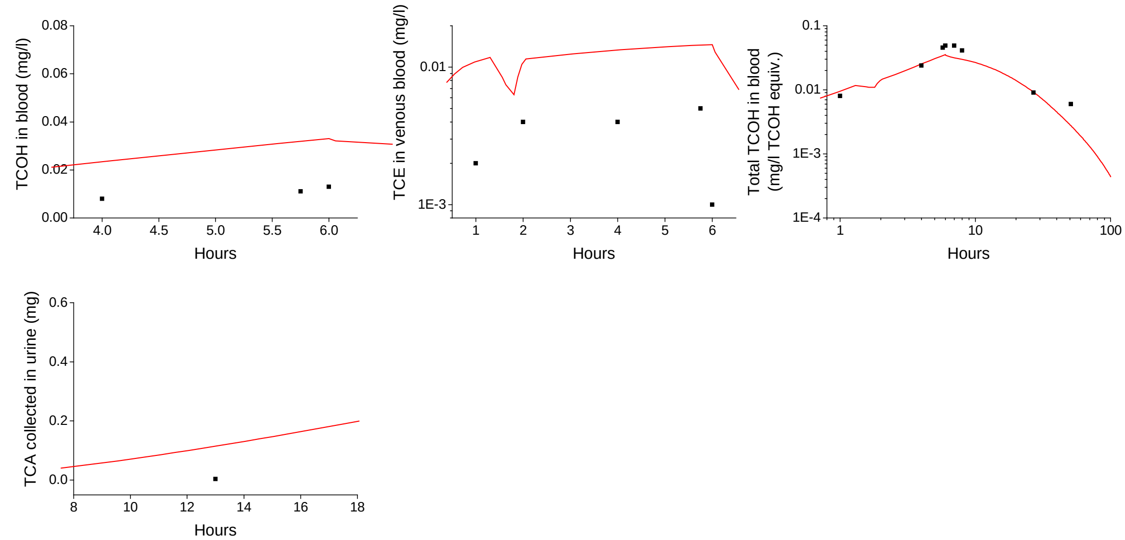
Chiu *et al.* 2007 Human #41 (sex=Male) – 1 ppm TCE 6 hour Inhalation



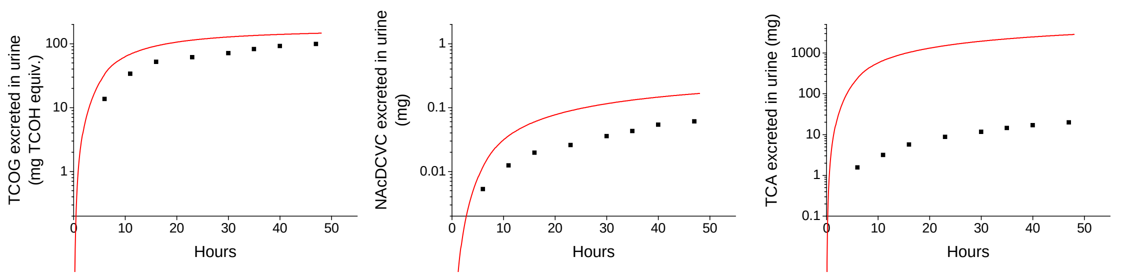
Chiu *et al.* 2007 Human #42 (sex=Male) – 1 ppm TCE 6 hour Inhalation



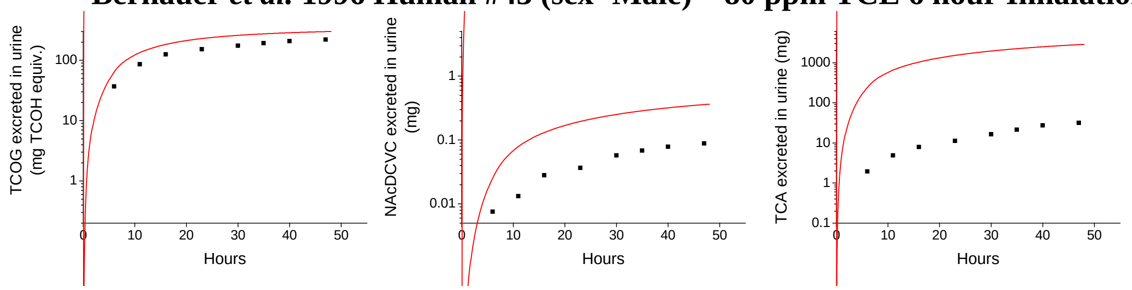
Chiu *et al.* 2007 Human #42 (sex=Male) – 1 ppm TCE 6 hour Inhalation



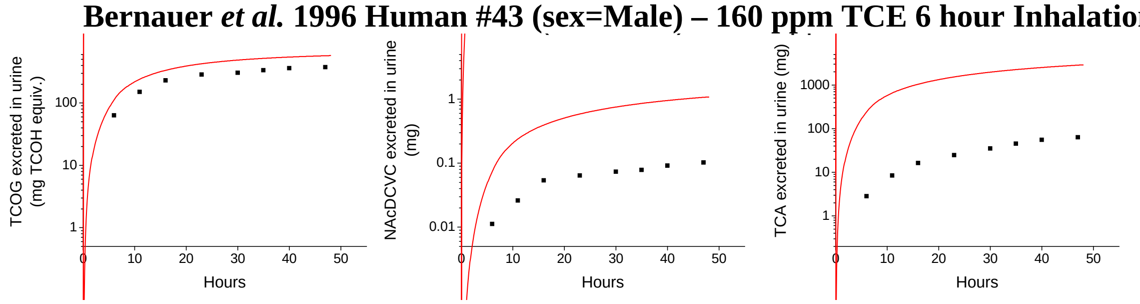
Bernauer *et al.* 1996 Human #43 (sex=Male) – 40 ppm TCE 6 hour Inhalation



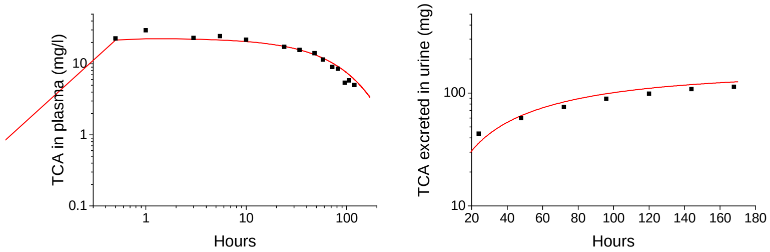
Bernauer *et al.* 1996 Human #43 (sex=Male) – 80 ppm TCE 6 hour Inhalation



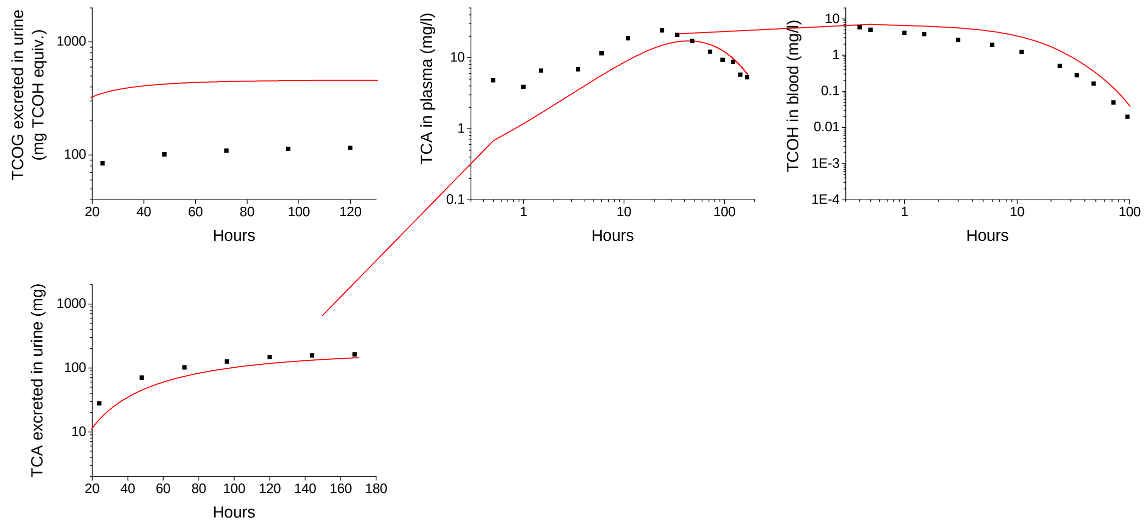
Bernauer *et al.* 1996 Human #43 (sex=Male) – 160 ppm TCE 6 hour Inhalation



Muller *et al.* 1974 Human #44 (sex=Male) – 2.646 mg/kg TCA Oral



Muller *et al.* 1974 Human #44 (sex=Male) – 10 mg/kg TCOH Oral



APPENDIX D. acslX MODEL CODE FOR 2011 EPA MODEL

Please note that some lines in this appendix carry over to a second line only because they were too long for the page width in Microsoft Word. These lines are not too long for single line acslX code in an actual CSL file and do not include continuation characters; therefore, the break in the lines will need to be removed for using this text if converted to a CSL file.

```
PROGRAM EPA_2011_TCE.csl
! acslX version of model from Appendix A of EPA Toxicological Review of TCE (September 2011)

! --- HISTORY OF HACK ET AL. (2006) MODEL
! Model code to correspond to the block diagram version of the harmonized model edited by Deborah
Keys to
!    incorporate Lapare et al. 1995 data -- Last edited: August 6, 2004
! Translated into MCSim from acslXtreme CSL file by Eric Hack, completed September 15, 2004
!   Removed non-essential differential equations (i.e., AUCCBld) for MCMC runs
!   Changed QRap and QSlw calculations and added QTot to scale fractional flows back to 1.0 after
sampling
! Changed QSlw calculation and removed QTot (September 21, 2004)
! Removed diffusion-limited fat uptake (September 24, 2004)

! --- HISTORY OF U.S. EPA (2009) MODEL (Chiu et al., 2009)
! Extensively revised by U.S. EPA June 2007 - June 2008
! Version 1
!   Fixed hepatic plasma flow for TCA-submodel to include portal vein (i.e., QGutLivPlas --
originally was
!      just QLivPlas, which was only hepatic artery)
!   Clearer coding and in-line documentation
!   Single model for 3 species
!   Revised physiological parameters, with discussion of uncertainty and variability
!   In vitro data used for default metabolism parameters, with discussion of uncertainty and
variability
!   Added
!      TCE blood compartment
!      TCE kidney compartment, with GSH metabolism
!      DCVG compartment
!      Additional outputs available from in vivo data
!      IA and PV dosing (for rats)
!   Removed DCA compartment
!
! Version 1.1 -- fixed urinary parameter scaling
!   Fixed VBod in kUrnTCOG (should be VBodTCOH)
!
! Version 1.1.1 -- changed some truncation limits (in commments only)
! Version 1.2
!   Removed TB compartment as currently coded
!   Added respiratory oxidative metabolism:  3 states:  AInhResp, AResp, AExhResp
!   Removed clearance from respiratory metabolism
!
! Version 1.2.1 -- changed oral dosing to be similar to IV
! Version 1.2.2 -- fixed default lung metabolism (additional scaling by lung/liver weight ratio)
! Version 1.2.3 -- fixed FracKidDCVC scaling


! --- Changes made in converting EPA model from MCSim to acslX
! Terms in some equations were rearranged for better readability
! Model changed to not use the parameter "Male" -- calculations didn't differ, only baseline
values for
!    parameters -- male and female specific M files created and those should be used
! Model changed to use absolute value rather than the baseline value times the fractional
increase
!    -- values in M files set accordingly (i.e., changed
PLivTCA=TCAPlas*exp(lnPLivTCAC)*(baseline
!    values) to PLivTCA=TCAPlas*PLivTCAC)
! Replaced "exp(ln*)" with "*" where "*" is the parameter name (i.e., replaced "exp(lnPBodTCAC)"
with
```

```
!    "PBodTCAC") -- "ln" removed from parameter names as appropriate
! Changed code to set measured values for BW, QP, VFatC, PB or Hematocrit in M file rather than
having
!    separate parameter for it and using IF statements to set
!    if Hematocrit measured, in the M file set FracPlas to (1-HematocritMeas) where
HematocritMeas is the
!       measured value
!    if QP is measured, in the M file set QCC to (QPMeas/VPR)/(BW^0.75) where QPMeas is the
measured value
!       -- not used in any of the M files
! QC used instead of QCNow since code was changed in how it uses measured QP values
! No fractional increase for QSlw since it is calculated in model but it does use a baseline
value for
!    total volume of perfused tissues so parameter VPerfC defined to be the baseline value
! New parameter defined for initial value for ACh called ACh0 since acslX handles initial values
for state
!    parameters differently than MCSim
! Use of "CC" for inhalation concentration for closed chamber changed to be used as a flag to
denote closed
!    chamber and concentration set with "CONC"
! AUrnTCA_sat, zAUrnTCA_sat, AUrnTCOG_sat and AUrnTCOGTCOH_sat are not used in any of the M files
so these
!    were removed since it was unclear what they should represent and how to recode them for
acslX

! Parameter "ConcOn" defined to turn inhalation dosing on and off -- used for acslX
implementation of
!    inhalation dosing but not needed for MCSim
! Equation for CInhPPM changed from "ACh/VCh*24450.0/MWTCE" to "(CInh*24450.0)/MWTCE" which would
be the
!    same results for closed chamber inhalation since CInh is defined as "ACh/VCh" which is the
only time
!    this endpoint is used but changing the equation this way allows the equation to work for
either closed
!    or open chamber
! Changed equation for AExhExp -- instead of "AExhExp=INTEG(RAExh, 0.0)" used "AExhExp=AExh"
! Code for calculating AUrnTCA_Coll changed to work better in acslX
! Added code for weekly and daily average dosemetrics
! Added parameters Days and TMax for repeated dosing

! Q*Ctmp renamed to Q*C where * is for the tissue (Fat, Gut, Kid, Liv, or Slw)
! DResptmp renamed DRespC
! VRespEffC renamed VRespC
! VRespEfftmp renamed VResp
! ClC renamed Cl (became ClC after removing "exp(ln" from equations)
! ClDCVGC renamed ClDCVG (became ClDCVGC after removing "exp(ln" from equations)
! ClKidDCVGC renamed ClKidDCVG (became ClKidDCVGC after removing "exp(ln" from equations)
! VMaxLungLivC renamed VMaxLungLiv (became VMaxLungLivC after removing "exp(ln" from equations)
! ClTCOHC renamed ClTCOH (became ClTCOHC after removing "exp(ln" from equations)
! ClGlucC renamed ClGluc (became ClGlucC after removing "exp(ln" from equations)
! ExhFactor_den renamed ExhFac_den
! CPlasTCAMole and CPlasTCAFreeMole renamed CPlasTCA_uMole and CPlasTCAFree_uMole, respectively,
since the
!    units are actually umoles
! RUrnTCA renamed RAUrnTCA
! RUrnTCOG renamed RAUrnTCOG
! RAMetDCVGmole renamed RAMetDCVG_Mole
! ADCVGmol renamed ADCVG_Mole
! CDCVGmol renamed CDCVG_Mole
! AMetDCVG renamed AMetDCVG_Mole
! CVenMole renamed CVen_Mole
! AUrnTCA_collect and zAUrnTCA_collect renamed AUrnTCA_Coll and zAUrnTCA_Coll, respectively
! AUrnTCOGTCOH_collect renamed AUrnTCOGTCOH_Coll

! AUrnTCTotMole renamed AUrnTCTot_Mole
! AUrnNDCVCequiv renamed AUrnNDCVC_Eq

! These parameters weren't used so they are not included in the acslX code (in alphabetical
order):
!    AUrnTCA_sat, AUrnTCOG_sat, AUrnTCOGTCOH_sat, CDCVGmolLD, CDCVG_NDtmp, CDCVG_ND, MWChlor,
QRapC,
```

```
!    RUrnNDCVC, RUrnTCOGTCOH, StochChlorTCE, StochTCEGluc, StochDCATCE, TCAUrnSat, TCOGUrnSat,
VBldCtmp,
!    VBodCtmp, VBodTCOHCtmp, VFatCtmp, VGutCtmp, VKidCtmp, VLivCtmp, VRapCtmp, VRespEffCtmp,
VRespLumCtmp,
!    VSlwCtmp, VPlasCtmp, zAUrnTCA_sat


INITIAL
  LOGICAL  CC, UrnMissing
  INTEGER  Species

  CONSTANT              BW = 0.0       ! Body weight (kg)
  CONSTANT             QCC = 1.0       ! Cardiac output (L/hr/kg^0.75)
  CONSTANT             VPR = 1.0       ! Alveolar ventilation-perfusion ratio (unitless)
  CONSTANT          DRespC = 1.0       ! Respiratory lumen/tissue diffusive clearance rate
(fraction of QP)



! Fractional Blood Flows to Tissues (fraction of cardiac output)
  CONSTANT           QFatC = 1.0       ! Fat
  CONSTANT           QGutC = 1.0       ! Gut
  CONSTANT           QKidC = 1.0       ! Kidney
  CONSTANT           QLivC = 1.0       ! Liver
  CONSTANT           QSlwC = 1.0       ! Slowly perfused tissues

! Tissue Volumes (fraction of body weight)
  CONSTANT           VBldC = 1.0       ! Blood
  CONSTANT           VFatC = 1.0       ! Fat
  CONSTANT           VGutC = 1.0       ! Gut
  CONSTANT           VKidC = 1.0       ! Kidney
  CONSTANT           VLivC = 1.0       ! Liver
  CONSTANT           VRapC = 1.0       ! Rapidly perfused tissues
  CONSTANT       VRespLumC = 1.0       ! Respiratory lumen
  CONSTANT          VRespC = 1.0       ! Respiratory tissue
  CONSTANT          VPerfC = 1.0       ! Body that is blood perfuse
  CONSTANT        FracPlas = 1.0       ! Fraction of blood that is plasma (1.0 - hematocrit)
(unitless)

! Molecular Weights (g/mole)
  CONSTANT           MWTCE = 131.39    ! TCE
  CONSTANT          MWDCVC = 216.1     ! DCVC
  CONSTANT           MWTCA = 163.5     ! TCA
  CONSTANT          MWTCOH = 149.5     ! TCOH
  CONSTANT      MWTCOHGluc = 325.53    ! TCOH-Gluc
  CONSTANT        MWNADCVC = 258.8     ! N Acetyl DCVC

! Partition Coefficients for TCE (unitless)
  CONSTANT              PB = 1.0       ! Blood/air
  CONSTANT            PFat = 1.0       ! Fat/blood
  CONSTANT            PGut = 1.0       ! Gut/blood
  CONSTANT            PKid = 1.0       ! Kidney/blood
  CONSTANT            PLiv = 1.0       ! Liver/blood
  CONSTANT            PRap = 1.0       ! Rapidly perfused/blood
  CONSTANT           PResp = 1.0       ! Respiratory tissue/air
  CONSTANT            PSlw = 1.0       ! Slowly perfused/blood

! Partition Coefficients for TCA
  CONSTANT     PRBCPlasTCA = 1.0       ! Scaled to species-specific central estimates (units ?)
  CONSTANT        PBodTCAC = 1.0       ! Free body/blood plasma (units ?)
  CONSTANT        PLivTCAC = 1.0       ! Free liver/blood plasma (units ?)
! Partition Coefficients for TCOH (unitless)
  CONSTANT        PBodTCOH = 1.0       ! Body/blood
  CONSTANT        PLivTCOH = 1.0       ! Liver/blood

! Partition Coefficients for TCOG (unitless)
  CONSTANT        PBodTCOG = 1.0       ! Body/blood
  CONSTANT        PLivTCOG = 1.0       ! Liver/blood

! Partition Coefficient for DCVG (unitless)
  CONSTANT        PEffDCVG = 1.0       ! Effective PC for the "body" (non-blood) compartment
```

```
! Binding Parameters for TCA
  CONSTANT         BMaxkDC = 1.0       ! Protein concentration (umole/L)
  CONSTANT         kDissoc = 1.0       ! Protein/TCA dissociation constant (umole/L)

! Oral Uptake Constants (/hr)
  CONSTANT             kAS = 1.4       ! TCE stomach absorption coefficient
  CONSTANT            kTSD = 1.4       ! TCE stomach to duodenum transfer coefficient
  CONSTANT             kAD = 0.75      ! TCE duodenum absorption coefficient
  CONSTANT             kTD = 0.1       ! TCE duodenum-feces transfer coefficient
  CONSTANT          kASTCA = 0.75      ! TCA stomach absorption coefficient
  CONSTANT         kASTCOH = 0.75      ! TCOH stomach absorption coefficient

! TCE Metabolism Constants
  CONSTANT           VMaxC = 1.0       ! Capacity for hepatic TCE oxidation (mg/hr/kg liver)
  CONSTANT             KMC = 1.0       ! Affinity for hepatic TCE oxidation (mg/L)
  CONSTANT              Cl = 1.0       ! Ratio of capacity to affinity per kg liver for TCE
hepatic oxidation (L/hr/kg liver)
  CONSTANT        FracTCAC = 1.0       ! Fraction of hepatic TCE oxidation to TCA (unitless)
  CONSTANT      FracOtherC = 1.0       ! Fraction of hepatic TCE oxidation not to TCA and TCOH
(unitless)
  CONSTANT       VMaxDCVGC = 1.0       ! Capacity for hepatic TCE GSH conjugation (mg/hr/kg
liver)
  CONSTANT         KMDCVGC = 1.0       ! Affinity for hepatic TCE GSH conjugation (mg/L)
  CONSTANT          ClDCVG = 1.0       ! Ratio of capacity to affinity per kg liver for TCE GSH
conjugation (L/hr/kg liver)
  CONSTANT    VMaxKidDCVGC = 1.0       ! Capacity for renal TCE GSH conjugation (mg/hr/kg kidney)
  CONSTANT      KMKidDCVGC = 1.0       ! Affinity for renal TCE GSH conjugation (mg/L)
  CONSTANT       ClKidDCVG = 1.0       ! Ratio of capacity to affinity per kg kidney for TCE GSH
conjugation (L/hr/kg kidney)


! TCE Metabolsim Constants for Chloral Kinetics in Clara Cells in Lung
  CONSTANT  VMaxLungLiv = 1.0 ! Ratio of capacities for lung to liver, scaled central estimates
(unitless)
  CONSTANT      KMClara = 1.0 ! Affinity for tracheo-bronchial TCE oxidation (in units of air
conc) (mg/L)
  CONSTANT FracLungSysC = 1.0 ! Frac of resp. oxidative metabolism entering systemic circulation
(unitless)

! TCOH Metabolism Constants
  CONSTANT       VMaxTCOHC = 1.0    ! Capacity for hepatic clearance of TCOH to TCA
(mg/hr/kg^0.75)
  CONSTANT          KMTCOH = 1.0    ! Affinity for hepatic clearance of TCOH to TCA (mg/L)
  CONSTANT          ClTCOH = 1.0    ! ??? (scaled by BW^0.75)
  CONSTANT       VMaxGlucC = 1.0    ! Capacity for hepatic glucuronidation of TCOH to TCOG
(mg/hr/kg^0.75)
  CONSTANT          KMGluc = 1.0    ! Affinity for hepatic glucuronidation of TCOH to TCOG (mg/L)
  CONSTANT          ClGluc = 1.0    ! ??? (scaled by BW^0.75)
  CONSTANT       kMetTCOHC = 1.0    ! Rate constant for hepatic clearance of TCOH to other
(kg^0.25/hr)

! TCA Metabolism and Clearance Rates
  CONSTANT        kUrnTCAC = 1.0  ! Rate constant for urinary clearance of TCA in plasma to urine
(L/hr-kg)
  CONSTANT        kMetTCAC = 1.0  ! Rate constant for hepatic clearance of TCA to other
(kg^0.25/hr)

! TCOG Metabolism and Clearance Rates
  CONSTANT          kBileC = 1.0      ! Rate constant for excretion of TCOG in liver to bile
(kg^0.25/hr)
  CONSTANT           kEHRC = 1.0      ! Lumped rate constant for TCOG in bile to TCOH in liver
(kg^0.25/hr)
  CONSTANT       kUrnTCOGC = 1.0      ! Rate constant for excretion of TCOG in urine (L/hr/kg)

! DCVG Metabolism Rates
  CONSTANT          kDCVGC = 1.0  ! Rate constant for hepatic clearance of DCVG to DCVC
(kg^0.25/hr)
  CONSTANT    FracKidDCVCC = 1.0  ! Frac of renal TCE GSH conj "directly" to DCVC (ie, 1st pass)
(unitless)
```

```
! DCVC Metabolism and Clearance Rates (kg^0.25/hr)
  CONSTANT           kNATC = 1.0  ! Lumped rate constant for DCVC clearance to urinary NAcDCVC
(kg^0.25/hr)
  CONSTANT     kKidBioactC = 1.0  ! Rate constant for other bioactivation of DCVC (kg^0.25/hr)

! Closed Chamber Parameters
  CONSTANT              CC = .FALSE.   ! Default to open chamber
  CONSTANT        NRodents = 1.0       ! Number of rodents in the chamber
  CONSTANT          kLossC = 1.0       ! Rate constant for closed chamber air loss (/hr)
  CONSTANT            VChC = 1.0       ! Volume of the chamber without animals (L)

! TCE Dosing Parameters
  CONSTANT            Conc = 0.0       ! Inhalation exposure concentration (ppm)
  CONSTANT          IVDose = 0.0       ! IV dose (mg/kg/day)
  CONSTANT           TChng = 0.003     ! IV infusion duration (hrs)
  CONSTANT            Days = 1.0       ! Days of exposure each week
  CONSTANT            TMax = 24.0      ! Maximum length of multiple exposures (hrs)
  CONSTANT           PDose = 0.0       ! Oral dose (mg/kg/day)
  CONSTANT           Drink = 0.0       ! Drinking water dose (mg/kg/day)
  CONSTANT          IADose = 0.0       ! Intraarterial dose (mg/kg)
  CONSTANT          PVDose = 0.0       ! Portal vein dose (mg/kg)

! TCA Dosing Parameters
  CONSTANT       IVDoseTCA = 0.0       ! IV dose of TCA (mg/kg/day)
  CONSTANT       PODoseTCA = 0.0       ! Oral dose of TCA (mg/kg/day)

! TCOH Dosing Parameters
  CONSTANT      IVDoseTCOH = 0.0       ! IV dose of TCOH (mg/kg/day)
  CONSTANT      PODoseTCOH = 0.0       ! Oral dose of TCOH (mg/kg/day)

! Flags for Species and Sex
  CONSTANT         Species = 1         ! 1=human, 2=rat, 3=mouse
  CONSTANT      UrnMissing = .FALSE.   ! Flag for missing urine collection times
  CONSTANT       CollectTm = 100000.0  ! Time to start collection for urine collection (hrs)
  CONSTANT      CollectInt = 100000.0  ! Collection interval for urine collection (hrs)

! Simulation Control Parameters
  CONSTANT          AvgInt = 168.0     ! Time period for calculating daily or weekly dosemetrics
  CONSTANT            TStp = 24.0      ! Time to stop simulation (hrs)
  CINTERVAL           CINT = 0.01

! Scaled Flow Rates (L/hr)
            QC = QCC * (BW**0.75)
            QP = QC * VPR
            QM = QP / 0.7              ! Minute-volume
         DResp = DRespC * QP

! Blood Flows to Tissues (L/hr)
          QFat = QFatC * QC
          QGut = QGutC * QC
          QKid = QKidC * QC
          QLiv = QLivC * QC
       QGutLiv = QGut + QLiv
          QSlw = QSlwC * QC
          QRap = QC - QFat - QGut - QKid - QLiv - QSlw
          QBod = QC - QGutLiv
! Plasma Flows to Tissues (L/hr)
        QCPlas = FracPlas * QC
      QBodPlas = FracPlas * QBod
   QGutLivPlas = FracPlas * QGutLiv

! Tissue Volumes (L)
          VBld = VBldC * BW
         VPlas = FracPlas * VBld
          VFat = VFatC * BW
          VGut = VGutC * BW
          VKid = VKidC * BW
          VLiv = VLivC * BW
          VRap = VRapC * BW
      VRespLum = VRespLumC * BW
```

```
        VResp = VRespC * BW
     VRespEff = VResp * PResp * PB    ! Effective respiratory tissue (L air) = V(tissue) *
Resp:Air partition coefficient
         VSlw = (VPerfC * BW) - VBld - VFat - VGut - VKid - VLiv - VRap - VResp
         VBod = VFat + VGut + VKid + VRap + VResp + VSlw
     VBodTCOH = VBld + VBod
        VDCVG = VBld + (PEffDCVG * (VBod + VLiv))

! Stoichiometry
   StochTCATCE = MWTCA / MWTCE
  StochTCATCOH = MWTCA / MWTCOH
  StochTCOHTCE = MWTCOH / MWTCE
 StochGlucTCOH = MWTCOHGluc / MWTCOH
 StochTCOHGluc = MWTCOH / MWTCOHGluc
  StochDCVCTCE = MWDCVC / MWTCE
        StochN = MWNADCVC / MWDCVC

! Partition Coefficients for TCA
       TCAPlas = FracPlas + ((1.0 - FracPlas) * PRBCPlasTCA)
       PBodTCA = TCAPlas * PBodTCAC
       PLivTCA = TCAPlas * PLivTCAC

! Binding Parameters for TCA
          BMax = kDissoc * BMaxkDC



! TCE Metabolism Constants (scale some parameters differently for humans than for mice and rats)
          VMax = VMaxC * VLiv
     FracOther = FracOtherC / (1.0 + FracOtherC)
       FracTCA = (FracTCAC * (1.0 - FracOther)) / (1.0 + FracTCAC)

  IF (Species .EQ. 1) THEN
      KM = VMax / (VLiv * Cl)
      VMaxDCVG = VLiv * ClDCVG * KMDCVGC
      KMDCVG = KMDCVGC
      VMaxKidDCVG = VKid * ClKidDCVG * KMKidDCVGC
      KMKidDCVG = KMKidDCVGC
  ELSE
      KM = KMC
      VMaxDCVG = VMaxDCVGC * VLiv
      KMDCVG = VMaxDCVG / (VLiv * ClDCVG)
      VMaxKidDCVG = VMaxKidDCVGC * VKid
      KMKidDCVG = VMaxKidDCVG / (VKid * ClKidDCVG)
  ENDIF

! TCE Metabolism Constants for Chloral Kinetics in Lung (mg/hr)
     VMaxClara = VMaxLungLiv * VMax
   FracLungSys = FracLungSysC / (1.0 + FracLungSysC)

! TCOH Metabolism Constants (mg/hr) (scale some parameters differently for humans than for mice
and rats)
      kMetTCOH = kMetTCOHC / (BW**0.25)

  IF (Species .EQ. 1) THEN
      VMaxTCOH = ClTCOH * KMTCOH * (BW**0.75)
      VMaxGluc = ClGluc * KMGluc * (BW**0.75)
  ELSE
      VMaxTCOH = VMaxTCOHC * (BW**0.75)
      VMaxGluc = VMaxGlucC * (BW**0.75)
  ENDIF

! TCA Metabolism and Clearance Rates
       kUrnTCA = (kUrnTCAC * BW) / VPlas
       kMetTCA = kMetTCAC / (BW**0.25)

! TCOG Metabolism and Clearance Rates
         kBile = kBileC / (BW**0.25)

          kEHR = kEHRC / (BW**0.25)
      kUrnTCOG = (kUrnTCOGC * BW) / (VBodTCOH * PBodTCOG)
```

```
! DCVG Metabolism Rates
         kDCVG = kDCVGC / (BW**0.25)
   FracKidDCVC = FracKidDCVCC / (1.0 + FracKidDCVCC)

! DCVC Metabolism and Clearance Rates (kg^0.25/hr)
          kNAT = kNATC / (BW**0.25)
    kKidBioact = kKidBioactC / (BW**0.25)

! Exposure definition
  IF (CC) THEN
      Rodents = NRodents                         ! Closed chamber simulation
      kLoss = kLossC
      VCh = VChC - (Rodents * BW)                ! Calculate net chamber volume
  ELSE
      Rodents = 0.0                              ! Open chamber simulation
      kLoss = 0.0                                ! Turn off chamber losses so concentration is
constant
      VCh = 1.0                                  ! So that VCh drops out of equations
  ENDIF
        ACh0 = (Conc * VCh * MWTCE) / 24450.0    ! Initial amount in chamber

! Initialize starting value
         Day = 0.5
      ConcOn = 0.0
        CInh = 0.0
         kIV = 0.0
      kIVTCA = 0.0
     kIVTCOH = 0.0
      kDrink = (Drink * BW) / 24.0             ! Ingestion rate via drinking water (mg/hr)
         kIA = 0.0
         kPV = 0.0
       kStom = 0.0
    kStomTCA = 0.0
   kStomTCOH = 0.0
     AExhExp = 0.0
    PAUCCBld = 0.0
  PAUCLivTCA = 0.0
   PAUCCTCOH = 0.0
   AUCCBldDM = 0.0
 AUCLivTCADM = 0.0
  AUCCTCOHDM = 0.0
  AUrnTCA_Coll = 0.0
 AUrnTCOG_Coll = 0.0

  SCHEDULE Calc .AT. TStp-AvgInt
  IF (UrnMissing) SCHEDULE StrtColl .AT. CollectTm
END


DYNAMIC
  ALGORITHM IALG = 2

DISCRETE DoseOn
  INTERVAL DoseInt = 10000.0                     ! Dosing interval (hrs)
  SCHEDULE DoseOff .AT. T + TChng

  IF ((T .LT. TMax) .AND. (Day .LE. Days)) THEN
       kIV = (IVDose * BW) / TChng               ! TCE IV infusion rate (mg/hr)
       kIVTCA = (IVDoseTCA * BW) / TChng         ! TCA IV infusion rate (mg/hr)
       kIVTCOH = (IVDoseTCOH * BW) / TChng       ! TCOH IV infusion rate (mg/hr)
       kIA = (IADose * BW) / TChng               ! IA infusion rate (mg/hr)
       kPV = (PVDose * BW) / TChng               ! PV infusion rate (mg/hr)
       ConcOn = 1.0
       kStom = (PDose * BW) / TChng              ! PO dose rate (into stomach) (mg/hr)
       kStomTCA = (PODoseTCA * BW) / TChng       ! TCA PO dose rate into stomach (mg/hr)
       kStomTCOH = (PODoseTCOH * BW) / TChng     ! TCOH PO dose rate into stomach (mg/hr)
  ENDIF

  Day = Day + 1.0
  IF (Day.GT.7.0) Day = 0.5
```

```
END

DISCRETE DoseOff
  kIV = 0.0
  kIVTCA = 0.0
  kIVTCOH = 0.0
  kIA = 0.0
  kPV = 0.0
  kStom = 0.0
  kStomTCA = 0.0
  kStomTCOH = 0.0
  ConcOn = 0.0
END

DISCRETE Calc
! Save previous value for calculating daily or weekly dosemetrics
  PAUCCBld = AUCCBld
  PAUCLivTCA = AUCLivTCA
  PAUCCTCOH = AUCCTCOH
END

DISCRETE StrtColl
! Save previous value for amount in urine
  PAUrnTCA = AUrnTCA
  PAUrnTCOG = AUrnTCOG
  SCHEDULE EndColl .AT. T + CollectInt
END

DISCRETE EndColl
! Save amount collected in urine for collection period
  AUrnTCA_Coll = AUrnTCA - PAUrnTCA
  AUrnTCOG_Coll = AUrnTCOG - PAUrnTCOG
END


! ------- TCE Output Variables -----------------------------------------------------------------
----------! Amount metabolized in the effective respiratory tissue (mg)
 AMetLngBW34 = AMetLng / (BW**0.75)
 AMetLngResp = AMetLng / VResp

! Amount of TCE in rapidly perfused tissues (mg)
        CHrt = CRap
       CLung = CRap
        CSpl = CRap
        CBrn = CRap

  PROCEDURAL (CMus = CSlw)
    CMus = CSlw
    IF (CSlw .LT. 1.0e-15) CMus = 1.0e-15
  END

! Amount of TCE metabolized to TCA, DCA and TCOH in liver (mg)
    AMetLivOther = AMetLiv1 * FracOther
         AMetGSH = AMetLiv2 + AMetKid
     AMetGSHBW34 = AMetGSH / (BW**0.75)
    AMetLiv1BW34 = AMetLiv1 / (BW**0.75)
AMetLivOtherBW34 = AMetLivOther / (BW**0.75)
     AMetLiv1Liv = AMetLiv1 / VLiv
 AMetLivOtherLiv = AMetLivOther / VLiv

! Concentration of TCE in mixed venous blood (mg/L)
   CVen_Mole = CVen / MWTCE
     CBldMix = (CArt + CVen) / 2.0


! ------- TCA Output Variables -----------------------------------------------------------------
----------
! Amount of TCA in the body (mg)
       CKidTCA = CBodTCA
      CLungTCA = CBodTCA
```

```
! Amount of TCA in urine (mg)
  PROCEDURAL (zAUrnTCA_Coll = AUrnTCA_Coll)
    zAUrnTCA_Coll = AUrnTCA_Coll
    IF (AUrnTCA_Coll .LT. 1.0e-15) zAUrnTCA_Coll = 1.0e-15
  END


! ------- TCOH Output Variables ----------------------------------------------------------
! Amount of TCOH in the body (mg)
      CKidTCOH = CBodTCOH
     CLungTCOH = CBodTCOH

! Amount of TCOH-Gluc in the body (mg)
  PROCEDURAL (CBodTCOGTCOH = VBodTCOH, StochTCOHGluc)
    CBodTCOGTCOH = StochTCOHGluc * (ABodTCOG / VBodTCOH)
    IF (ABodTCOG .LT. 1.0e-15) CBodTCOGTCOH = 1.0e-15
  END

  CKidTCOGTCOH = CBodTCOGTCOH
 CLungTCOGTCOH = CBodTCOGTCOH


! Amount of TCOH-Gluc in liver (mg)
  PROCEDURAL (CLivTCOGTCOH = VLiv, StochTCOHGluc)
    CLivTCOGTCOH = StochTCOHGluc * (ALivTCOG / VLiv)
    IF (ALivTCOG .LT. 1.0e-15) CLivTCOGTCOH = 1.0e-15
  END


! ------- TCOG Output Variables ----------------------------------------------------------
! Total amount of TCOH-Gluc in tissues (mg)
         ATCOG = ABodTCOG + ALivTCOG

! Amount of TCOH-Gluc excreted in urine (mg)
  PROCEDURAL (AUrnTCOGCOH = StochTCOHGluc)
    AUrnTCOGTCOH = StochTCOHGluc * AUrnTCOG
    IF (AUrnTCOG .LT. 1.0e-15) AUrnTCOGTCOH = 1.0e-15
  END

  PROCEDURAL (AUrnTCOGTCOH_Coll = StochTCOHGluc, AUrnTCOG_Coll)
    AUrnTCOGTCOH_Coll = StochTCOHGluc * AUrnTCOG_Coll
    IF (AUrnTCOG_Coll .LT. 1.0e-15) AUrnTCOGTCOH_Coll = 1.0e-15
  END

! Total amount of TCOH and TCOH-Gluc (mg)
  TotCTCOHComp = CTCOH + CTCOG

! Total amount of TCA and TCOG in urine (mg)
AUrnTCTot_Mole = (zAUrnTCA / MWTCA) + (AUrnTCOGTCOH / MWTCOH)


! ------- DCVC Output Variables ----------------------------------------------------------
! Amount of DCVC in kidney (mg)
 ABioactDCVCBW34 = ABioactDCVC / (BW**0.75)
  ABioactDCVCKid = ABioactDCVC / VKid

! Amount of N Acetyl DCVC excreted (mg)
 AUrnNDCVC_Eq = AUrnNDCVC / StochN

  PROCEDURAL (zAUrnNDCVC = AUrnNDCVC)
    zAUrnNDCVC = AUrnNDCVC
    IF (AUrnNDCVC .LT. 1.0e-15) zAUrnNDCVC = 1.0e-15
  END
! ------- Mass Balance Equations ---------------------------------------------------------
! TCE
   TotTissue = AInhResp + AExhResp + AResp + AFat + AGut + AKid + ALiv + ARap + ASlw + ABld
    TotMetab = AMetLng + AMetKid + ATotMetLiv
     TCEDiff = TotDose - TotTissue - TotMetab
  MassBalTCE = TCEDiff - AExc - AExh
 TotDoseBW34 = TotDose / (BW**0.75)
TotMetabBW34 = TotMetab / (BW**0.75)
```

```
TotOxMetBW34 = (AMetLng + AMetLiv1) / (BW**0.75)

! TCA
  TotTissueTCA = APlasTCA + ABodTCA + ALivTCA
       TCADiff = TotTCAIn - TotTissueTCA - AMetTCA
    MassBalTCA = TCADiff - AUrnTCA
    TotTCAInBW = TotTCAIn / BW

! TCOH
     TotTissueTCOH = ABodTCOH + ALivTCOH
      TotMetabTCOH = AMetTCOHTCA + AMetTCOHGluc + AMetTCOHOther
       MassBalTCOH = TotTCOHIn - TotTissueTCOH - TotMetabTCOH
       TotTCOHDose = AOTCOH + ((1.0 - FracOther - FracTCA)*StochTCOHTCE*(AMetLiv1 +
(FracLungSys*AMetLng)))

! TCOG
     TotTCOGIn = StochGlucTCOH * AMetTCOHGluc
 TotTissueTCOG = ABodTCOG + ALivTCOG + ABileTCOG
   MassBalTCOG = TotTCOGIn - TotTissueTCOG - ARecircTCOG - AUrnTCOG

! DCVC
   MassBalDCVC = ADCVCIn - ADCVC - ABioactDCVC - AUrnNDCVC_Eq

! DCVG
   MassBalDCVG = ADCVGIn - ADCVG_Mole - AMetDCVG_Mole


DERIVATIVE
       Hours = T

! ------- TCE Model -----------------------------------------------------------------------------
! Amount of TCE in inhaled air (mg)
         ACh = INTEG(((Rodents * (QM * (CMixExh - (ACh / VCh)))) - (kLoss * ACh)), ACh0)

  PROCEDURAL (CInh = ConcOn, VCh)
    CInh = (Conc * MWTCE / 24450.0) * ConcOn
    IF (CC) CInh = (ACh / VCh) * ConcOn
  END
  PROCEDURAL (CInhPPM = CInh)
    CInhPPM = (CInh * 24450.0) / MWTCE
    IF (ACh .LT. 1.0e-15) CInhPPM = 1.0e-15
  END

! Amount of TCE in respiratory lumen (mg)
    AInhResp = INTEG(((QM * (CInh - CInhResp)) + (DResp * (CResp - CInhResp))), 0.0)
    CInhResp = AInhResp / VRespLum

! Concentration in mixed exhaled air (mg/L)
    AExhResp = INTEG(((QM * (CInhResp - CExhResp)) + (QP * ((CArt_Tmp / PB) - CInhResp))
             + (DResp * (CResp - CExhResp))), 0.0)
    CExhResp = AExhResp / VRespLum

  PROCEDURAL (CMixExh = CExhResp)
    CMixExh = 1.0e-15
    IF (CExhResp .GT. 0.0) CMixExh = CExhResp
  END

! Amount of TCE in the effective respiratory tissue (mg)
       AResp = INTEG(((DResp * (CInhResp + CExhResp - (2.0 * CResp))) - RAMetLng), 0.0)
       CResp = AResp / VRespEff

! Amount metabolized in the effective respiratory tissue (mg)
    RAMetLng = (VMaxClara * CResp) / (KMClara + CResp)
     AMetLng = INTEG(RAMetLng, 0.0)

! Concentration in arterial blood (mg/L)
    CArt_Tmp = ((QC * CVen) + (QP * CInhResp)) / (QC + (QP / PB))
     AUCCBld = INTEG(CArt, 0.0)

  PROCEDURAL (CArt = QC, CArt_Tmp, kIA)
    CArt = CArt_Tmp + (kIA / QC)
```

```
    IF (CArt .LT. 1.0e-15) CArt = 1.0e-15
  END


! Concentration in alveolar air (mg/L)
        CAlv = (CArt_Tmp / PB) * ExhFactor
  ExhFac_Den = (QP * (CArt_Tmp / PB)) + ((QM - QP) * CInhResp)


  PROCEDURAL (CAlvPPM = CAlv)
    CAlvPPM = CAlv * (24450.0 / MWTCE)
    IF (CAlv .LT. 1.0e-15) CAlvPPM = 1.0e-15
  END

  PROCEDURAL (ExhFactor = QM, CMixExh, ExhFac_Den)
    ExhFactor = 1.0
    IF (ExhFac_Den .GT. 0.0) ExhFactor = (QM * CMixExh) / ExhFac_Den
  END

! Amount exhaled (mg)
       RAExh = QM * CMixExh
        AExh = INTEG(RAExh, 0.0)

  PROCEDURAL (zAExh = AExh)
    zAExh = AExh
    IF (AExh .LT. 1.0e-15) zAExh = 1.0e-15
  END

  PROCEDURAL (AExhExp = CInh)
    AExhExp = 0.0
    IF (CInh .GT. 0.0) AExhExp = AExh
  END

  PROCEDURAL (zAExhPost = AExhExp)
    zAExhPost = AExh - AExhExp
    IF ((AExh - AExhExp) .LT. 1.0e-15) zAExhPost = 1.0e-15
  END

! Amount of TCE in fat tissue (mg)
        AFat = INTEG((QFat * (CArt - CVFat)), 0.0)
       CVFat = CFat / PFat

  PROCEDURAL (CFat = VFat)
    CFat = AFat / VFat

    IF (CFat .LT. 1.0e-15) CFat = 1.0e-15
  END

! Amount of TCE in stomach -- for oral dosing only (mg)
       AStom = INTEG((kStom - (kAS * AStom) - (kTSD * AStom)), 0.0)

! Amount of TCE in duodenum -- for oral dosing only (mg)
       ADuod = INTEG(((kTSD * AStom) - (kAD * ADuod) - (kTD * ADuod)), 0.0)

! Amount of TCE excreted in feces (mg)
       RAExc = kTD * ADuod
        AExc = INTEG(RAExc, 0.0)

! Amount of TCE absorbed (mg)
         RAO = kDrink + (kAS * AStom) + (kAD * ADuod)

! Amount of TCE in gut compartment (mg)
        AGut = INTEG(((QGut * (CArt - CVGut)) + RAO), 0.0)
       CVGut = CGut / PGut

  PROCEDURAL (CGut = VGut)
    CGut = AGut / VGut
    IF (CGut .LT. 1.0e-15) CGut = 1.0e-15
  END

! Amount of TCE in kidneys (mg)
```

```
        AKid = INTEG(((QKid * (CArt - CVKid)) - RAMetKid), 0.0)
       CVKid = CKid / PKid
     AUCCKid = INTEG(CKid, 0.0)

  PROCEDURAL (CKid = VKid)
    CKid = AKid / VKid
    IF (CKid .LT. 1.0e-15) CKid = 1.0e-15
  END

! Amount of TCE metabolized to DCVG in kidneys (mg)
    RAMetKid = (VMaxKidDCVG * CVKid) / (KMKidDCVG + CVKid)
     AMetKid = INTEG(RAMetKid, 0.0)

! Amount of TCE in liver (mg)
        ALiv = INTEG(((QLiv*(CArt - CVLiv)) + (QGut*(CVGut - CVLiv)) + kPV - RAMetLiv1 -
RAMetLiv2), 0.0)
       CVLiv = CLiv / PLiv
     AUCCLiv = INTEG(CLiv, 0.0)

  PROCEDURAL (CLiv = VLiv)
    CLiv = ALiv / VLiv

    IF (CLiv .LT. 1.0e-15) CLiv = 1.0e-15
  END

! Amount of TCE metabolized to TCA, DCA and TCOH in liver (mg)
   RAMetLiv1 = (VMax * CVLiv) / (KM + CVLiv)
    AMetLiv1 = INTEG(RAMetLiv1, 0.0)

! Amount of TCE metabolized to DCVG in liver (mg)
   RAMetLiv2 = (VMaxDCVG * CVLiv) / (KMDCVG + CVLiv)
    AMetLiv2 = INTEG(RAMetLiv2, 0.0)

! Total amount of TCE metabolized in liver (mg)
  ATotMetLiv = AMetLiv1 + AMetLiv2

! Amount of TCE in rapidly perfused tissues (mg)
        ARap = INTEG((QRap * (CArt - CVRap)), 0.0)
       CVRap = CRap / PRap
     AUCCRap = INTEG(CRap, 0.0)

  PROCEDURAL (CRap = VRap)
    CRap = ARap / VRap
    IF (CRap .LT. 1.0e-15) CRap = 1.0e-15
  END

! Amount of TCE in slowly perfused tissues
        ASlw = INTEG((QSlw * (CArt - CVSlw)), 0.0)
       CVSlw = CSlw / PSlw

  PROCEDURAL (CSlw = VSlw)
    CSlw = ASlw / VSlw
    IF (CSlw .LT. 1.0e-15) CSlw = 1.0e-15
  END

! Concentration of TCE in mixed venous blood (mg/L)
 ABld = INTEG(((QFat*CVFat + QKid*CVKid + QGutLiv*CVLiv + QRap*CVRap + QSlw*CVSlw + kIV) -
(QC*CVen)), 0.0)
  PROCEDURAL (CVen = VBld)
    CVen = ABld / VBld
    IF (CVen .LT. 1.0e-15) CVen = 1.0e-15
  END

! Total intake of TCE from all routes (mg)
    RInhDose = QM * CInh
     InhDose = INTEG(RInhDose, 0.0)
          AO = INTEG((RAO + kIV + kIA + kPV), 0.0)
     TotDose = InhDose + AO

  PROCEDURAL (RetDose = AExhExp)
    RetDose = 1.0e-15
```

```
    IF ((InhDose - AExhExp) .GT. 0.0) RetDose = InhDose - AExhExp
  END


! ------- TCA Sub-Model ---------------------------------------------------------------------
! Amount of TCA in plasma (mg)
      APlasTCA = INTEG(((QBodPlas*CVBodTCA)+(QGutLivPlas*CVLivTCA)+kIVTCA-(QCPlas*CPlasTCA)-
RAUrnTCA), 0.0)
    AUCPlasTCA = INTEG(CPlasTCA, 0.0)

  PROCEDURAL (CPlasTCA = VPlas)
    CPlasTCA = APlasTCA / VPlas
    IF ((APlasTCA .LT. 1.0e-15) .OR. (CPlasTCA .LT. 1.0e-15)) CPlasTCA = 1.0e-15
  END

  PROCEDURAL (CPlasTCA_uMole = CPlasTCA)
    CPlasTCA_uMole = (CPlasTCA / MWTCA) * 1000.0               ! (umole/L)
    IF (CPlasTCA_uMole .LT. 1.0e-15) CPlasTCA_uMole = 1.0e-15
  END

! Concentration of total TCA in blood (mg/L)
       CBldTCA = CPlasTCA * TCAPlas

! Concentration of free TCA in plasma in (umole/L)
             A = kDissoc + BMax - CPlasTCA_uMole
             B = 4.0 * kDissoc * CPlasTCA_uMole

  PROCEDURAL (C = A, B)
    C = SQRT((A**2.0) + B) - A
    IF (B .LT. (0.01 * (A**2.0))) C = B / 2.0 / A
  END

  PROCEDURAL (CPlasTCAFree_uMole = C)
    CPlasTCAFree_uMole = 0.5 * C
    IF (CPlasTCAFree_uMole .LT. 1.0e-15) CPlasTCAFree_uMole = 1.0e-15
  END

! Concentration of free TCA in plasma (mg/L)
  CPlasTCAFree = (CPlasTCAFree_uMole / 1000.0) * MWTCA
  APlasTCAFree = CPlasTCAFree * VPlas
AUCPlasTCAFree = INTEG(CPlasTCAFree, 0.0)

! Concentration of bound TCA in plasma (mg/L)
  PROCEDURAL (CPlasTCABnd = CPlasTCA, CPlasTCAFree)
    CPlasTCABnd = CPlasTCA - CPlasTCAFree
    IF (CPlasTCA .LT. CPlasTCAFree) CPlasTCABnd = 0.0
  END

! Amount of TCA in the body (mg)
       ABodTCA = INTEG((QBodPlas * (CPlasTCAFree - CVBodTCAFree)), 0.0)
  CVBodTCAFree = CBodTCA / PBodTCA
      CVBodTCA = CPlasTCABnd + CVBodTCAFree

  PROCEDURAL (CBodTCA = VBod)
    CBodTCA = ABodTCA / VBod
    IF (ABodTCA .LT. 0.0) CBodTCA = 0.0
    IF (CBodTCA .LT. 1.0e-15) CBodTCA = 1.0e-15
  END

! TCA oral absorption rate (mg/hr)
        kPOTCA = kASTCA * AStomTCA
      AStomTCA = INTEG((kStomTCA - (kASTCA * AStomTCA)), 0.0)

! Amount of TCA in the liver (mg)
       ALivTCA = INTEG(((QGutLivPlas*(CPlasTCAFree-CVLivTCAFree)) + kPOTCA  +
(StochTCATCOH*RAMetTCOHTCA)
               + (FracTCA*StochTCATCE*(RAMetLiv1 + (FracLungSys*RAMetLng))) - RAMetTCA), 0.0)
  CVLivTCAFree = CLivTCA / PLivTCA
      CVLivTCA = CPlasTCABnd + CVLivTCAFree
     AUCLivTCA = INTEG(CLivTCA, 0.0)
```

```
  PROCEDURAL (CLivTCA = VLiv)
    CLivTCA = ALivTCA / VLiv
    IF ((ALivTCA .LT. 1.0e-15) .OR. (CLivTCA .LT. 1.0e-15)) CLivTCA = 1.0e-15
  END

! Amount of TCA metabolized in liver (mg)
      RAMetTCA = kMetTCA * ALivTCA
       AMetTCA = INTEG(RAMetTCA, 0.0)

! Amount of TCA in urine (mg)
      RAUrnTCA = kUrnTCA * APlasTCAFree
       AUrnTCA = INTEG(RAUrnTCA, 0.0)

  PROCEDURAL (zAUrnTCA = AUrnTCA)
    zAUrnTCA = AUrnTCA
    IF (AUrnTCA .LT. 1.0e-15) zAUrnTCA = 1.0e-15
  END

! Total intake of TCA from all routes (mg)
         AOTCA = INTEG((kIVTCA + kPOTCA), 0.0)
      TotTCAIn = AOTCA + (FracTCA * StochTCATCE * (AMetLiv1 + (FracLungSys * AMetLng))) +
(StochTCATCOH * AMetTCOHTCA)


! ------- TCOH Sub-Model -----------------------------------------------------------------
! Concentration of TCOH (mg/L)
      AUCCTCOH = INTEG(CTCOH, 0.0)

  PROCEDURAL (CTCOH = QC, QBod, QGutLiv, CVBodTCOH, CVLivTCOH, kIVTCOH)
    CTCOH = (QBod*CVBodTCOH + QGutLiv*CVLivTCOH + kIVTCOH) / QC
    IF (CTCOH .LT. 1.0e-15) CTCOH = 1.0e-15
  END

! Amount of TCOH in the body (mg)
      ABodTCOH = INTEG((QBod * (CTCOH - CVBodTCOH)), 0.0)
     CVBodTCOH = ABodTCOH / VBodTCOH / PBodTCOH
   AUCCBodTCOH = INTEG((ABodTCOH / VBodTCOH), 0.0)

  PROCEDURAL (CBodTCOH = VBodTCOH)
    CBodTCOH = ABodTCOH / VBodTCOH

    IF (ABodTCOH .LT. 1.0e-15) CBodTCOH = 1.0e-15
  END

! TCOH oral absorption rate (mg/hr)
     AStomTCOH = INTEG((kStomTCOH - (kASTCOH * AStomTCOH)), 0.0)
       kPOTCOH = kASTCOH * AStomTCOH

! Amount of TCOH in liver (mg)
      ALivTCOH = INTEG(((QGutLiv*(CTCOH-CVLivTCOH)) + kPOTCOH + (StochTCOHGluc*RARecircTCOG)
               + ((1.0-FracOther-FracTCA)*StochTCOHTCE*(RAMetLiv1+(FracLungSys*RAMetLng)))
               - RAMetTCOH - RAMetTCOHTCA - RAMetTCOHGluc), 0.0)
     CVLivTCOH = ALivTCOH / VLiv / PLivTCOH

  PROCEDURAL (CLivTCOH = VLiv)
    CLivTCOH = ALivTCOH / VLiv
    IF (ALivTCOH .LT. 1.0e-15) CLivTCOH = 1.0e-15
  END

! Rate of oxidation to TCA (mg/hr)
  RAMetTCOHTCA = (VMaxTCOH * CVLivTCOH) / (KMTCOH + CVLivTCOH)
   AMetTCOHTCA = INTEG(RAMetTCOHTCA, 0.0)

! Amount of glucuronidation to TCOG (mg/hr)
 RAMetTCOHGluc = (VMaxGluc * CVLivTCOH) / (KMGluc + CVLivTCOH)
  AMetTCOHGluc = INTEG(RAMetTCOHGluc, 0.0)

! Amount of TCOH metabolized by other routes in liver (mg)
     RAMetTCOH = kMetTCOH * ALivTCOH
 AMetTCOHOther = INTEG(RAMetTCOH, 0.0)
        AOTCOH = INTEG((kIVTCOH + kPOTCOH), 0.0)
```

```
! Total intake of TCOH from all routes (mg)
         TotTCOHIn = AOTCOH + (StochTCOHGluc * ARecircTCOG) + ((1.0 - FracOther - FracTCA) *
StochTCOHTCE * (AMetLiv1 + (FracLungSys * AMetLng)))


! ------- TCOG Sub-Model ----------------------------------------------------------------------
! Concentration of TCOH-Gluc (mg/L)
  PROCEDURAL (CTCOG = QC, QBod, QGutLiv, CVBodTCOG, CVLivTCOG)
    CTCOG = (QBod*CVBodTCOG + QGutLiv*CVLivTCOG) / QC

    IF (CTCOG .LT. 1.0e-15) CTCOG = 1.0e-15
  END

! Amount of TCOH-Gluc in the body (mg)
      ABodTCOG = INTEG(((QBod * (CTCOG - CVBodTCOG)) - RAUrnTCOG), 0.0)
     CVBodTCOG = ABodTCOG / VBodTCOH / PBodTCOG

! Amount of TCOH-Gluc in liver (mg)
      ALivTCOG = INTEG(((QGutLiv*(CTCOG - CVLivTCOG)) + (StochGlucTCOH*RAMetTCOHGluc) -
RBileTCOG), 0.0)
     CVLivTCOG = ALivTCOG / VLiv / PLivTCOG

! Amount of TCOH-Gluc excreted into bile (mg)
     ABileTCOG = INTEG((RBileTCOG - RARecircTCOG), 0.0)
     RBileTCOG = kBile * ALivTCOG

  PROCEDURAL (zABileTCOG = ABileTCOG)
    zABileTCOG = ABileTCOG
    IF (ABileTCOG .LT. 1.0e-15) zABileTCOG = 1.0e-15
  END

! Amount of TCOH-Gluc recirculated (mg)
  RARecircTCOG = kEHR * ABileTCOG
   ARecircTCOG = INTEG(RARecircTCOG, 0.0)

! Amount of TCOH-Gluc excreted in urine (mg)
         RAUrnTCOG = kUrnTCOG * ABodTCOG
          AUrnTCOG = INTEG(RAUrnTCOG, 0.0)

! Total amount of TCOH and TCOH-Gluc (mg)
      TotCTCOH = CTCOH + CTCOGTCOH
   AUCTotCTCOH = INTEG(TotCTCOH, 0.0)

  PROCEDURAL (CTCOGTCOH = StochTCOHGluc, CTCOG)
    CTCOGTCOH = StochTCOHGluc * CTCOG
    IF (CTCOG .LT. 1.0e-15) CTCOGTCOH = 1.0e-15
  END


! ------- DCVC Sub-Model ---------------------------------------------------------------------
! Amount of DCVC in kidney (mg)
         ADCVCIn = INTEG(((RAMetDCVG_Mole * MWDCVC) + (FracKidDCVC * StochDCVCTCE * RAMetKid)),
0.0)
           ADCVC = INTEG(((RAMetDCVG_Mole * MWDCVC) + (FracKidDCVC * StochDCVCTCE * RAMetKid)
                 - (ADCVC * (kKidBioact + kNAT))), 0.0)
     ABioactDCVC = INTEG((kKidBioact * ADCVC), 0.0)

! Amount of DCVC excreted into urine (mg)
     RAUrnDCVC = kNAT * ADCVC

! Amount of N Acetyl DCVC excreted (mg)
    AUrnNDCVC = INTEG((StochN * RAUrnDCVC), 0.0)


! ------- DCVG Sub-Model ----------------------------------------------------------------------
! Amount of DCVG in kidney (mg)
       ADCVGIn = INTEG(((RAMetLiv2 + ((1.0 - FracKidDCVC) * RAMetKid)) / MWTCE), 0.0)

    ADCVG_Mole = INTEG((((RAMetLiv2 + ((1.0 - FracKidDCVC) * RAMetKid)) / MWTCE) -
RAMetDCVG_Mole), 0.0)
```

```
      AUCCDCVG = INTEG(CDCVG_Mole, 0.0)

  PROCEDURAL (CDCVG_Mole = VDCVG)
    CDCVG_Mole = ADCVG_Mole / VDCVG
    IF (CDCVG_Mole .LT. 1.0e-15) CDCVG_Mole = 1.0e-15
  END

! Amount of DCVG metabolized (mg)
RAMetDCVG_Mole = kDCVG * ADCVG_Mole
 AMetDCVG_Mole = INTEG(RAMetDCVG_Mole, 0.0)


  TERMT(T.GE.TStp, 'Simulation Finished')

END      ! of Derivative
END      ! of Dynamic


TERMINAL
! Calculate daily or weekly dosemetrics
     AUCCBldDM = AUCCBld - PAUCCBld
   AUCLivTCADM = AUCLivTCA - PAUCLivTCA
    AUCCTCOHDM = AUCCTCOH - PAUCCTCOH
END      ! of Terminal
END      ! of Program
```

APPENDIX E. M FILES FOR MOUSE SIMULATIONS

The following M files are for generating mouse output for validation figures in Appendix A.

Mouse.m

```
% Use posterior values

MousePost
```

MousePrior.m

```
% Parameters from Table A-4 (same as
baselines in model
%  code)
% DRespC, PEffDCVG, kAS, kTSD, kAD, kTD,
kASTCA, kASTCOH,
%  FracOtherC, KMClara, FracLungSysC,
VMaxTCOHC, KMTCOH,
%  VMaxGlucC, KMGluc, kMetTCOHC, kMetTCAC,
kBileC, kEHRC,
%  kDCVGC, FracKidDCVCC, kNATC, kKidBioactC
from
%  Table 3-37 in report

SPECIES=3;
BW=0.03; QCC=11.6; VPR=2.5; DRESPC=0.00813;
QFATC=0.07; QGUTC=0.141; QKIDC=0.091;
QLIVC=0.02; QSLWC=0.217;
VBLDC=0.049; VFATC=0.07; VGUTC=0.049;
VKIDC=0.017; VLIVC=0.055; VRAPC=0.1;
VRESPLUMC=0.004667; VRESPC=0.0007;
VPERFC=0.8897; FRACPLAS=0.52;
PB=15.0; PFAT=36.0; PGUT=1.9; PKID=2.1;
PLIV=1.7;
PRAP=1.9; PRESP=2.6; PSLW=2.4;
PRBCPLASTCA=0.5; PBODTCAC=0.88;
PLIVTCAC=1.18;
PBODTCOH=1.11; PLIVTCOH=1.3;
PBODTCOG=1.11; PLIVTCOG=1.3; PEFFDCVG=1.25;
BMAXKDC=0.88; KDISSOC=107.0;
KAS=1.7; KTSD=1.4; KAD=1.2; KTD=0.1;
KASTCA=0.63;
KASTCOH=0.75
VMAXC=2700.0; KMC=36.0; CL=1.0;
FRACTCAC=0.32;
FRACOTHERC=0.75;
VMAXDCVGC=300.0; KMDCVGC=1.0; CLDCVG=1.53;
VMAXKIDDCVGC=60.0; KMKIDDCVGC=1.0;
CLKIDDCVG=0.34;
VMAXLUNGLIV=0.07; KMCLARA=1.5;
FRACLUNGSYSC=0.52;
VMAXTCOHC=0.89; KMTCOH=1.4; CLTCOH=1.0;
VMAXGLUCC=1.53; KMGLUC=1.8; CLGLUC=1.0;
KMETTCOHC=0.079;
KURNTCAC=0.6; KMETTCAC=0.05;
KBILEC=0.13; KEHRC=0.087; KURNTCOGC=0.6;
KDCVGC=0.1; FRACKIDDCVCC=1.9;
KNATC=0.12; KKIDBIOACTC=0.075;
```

MousePost.m

```
% Parameters using baseline from Table A-4
(same as
%  baselines in model code) and posterior
changes in
%  Table A-9
% Baselines for DRespC, PEffDCVG, kAS, kTSD,
kAD, kTD,
%  kASTCA, kASTCOH, FracOtherC, KMClara,
FracLungSysC,
%  VMaxTCOHC, KMTCOH, VMaxGlucC, KMGluc,
kMetTCOHC,
%  kMetTCAC, kBileC, kEHRC, kDCVGC,
FracKidDCVCC, kNATC,
%  kKidBioactC from Table 3-37 in report

SPECIES=3;
BW=0.03; QCC=14.3; VPR=2.0; DRESPC=1.214;
QFATC=0.072; QGUTC=0.17; QKIDC=0.091;
QLIVC=0.021;
QSLWC=0.21;
VBLDC=0.049; VFATC=0.093; VGUTC=0.048;
VKIDC=0.017;
VLIVC=0.044; VRAPC=0.0997; VRESPLUMC=0.0047;
VRESPC=0.0007; VPERFC=0.8897; FRACPLAS=0.45;
PB=14.0; PFAT=35.0; PGUT=1.5; PKID=2.7;
PLIV=2.2;
PRAP=1.8; PRESP=2.6; PSLW=2.2;
PRBCPLASTCA=1.2; PBODTCAC=0.78;
PLIVTCAC=0.94;
PBODTCOH=0.89; PLIVTCOH=1.98;
PBODTCOG=0.47; PLIVTCOG=1.3; PEFFDCVG=1.0;
BMAXKDC=1.1; KDISSOC=130.0;
KAS=1.7; KTSD=5.2; KAD=0.27; KTD=0.1;
KASTCA=4.0;
KASTCOH=0.73;
VMAXC=1807.0; KMC=2.6; CL=1.0;
FRACTCAC=0.16;
FRACOTHERC=0.024;
VMAXDCVGC=455.0; KMDCVGC=1.0; CLDCVG=0.27;
VMAXKIDDCVGC=85.0; KMKIDDCVGC=1.0;
CLKIDDCVG=0.28;
VMAXLUNGLIV=0.203; KMCLARA=0.011;
FRACLUNGSYSC=3.3;
VMAXTCOHC=1.6; KMTCOH=0.96; CLTCOH=1.0;
VMAXGLUCC=66.0; KMGLUC=31.0; CLGLUC=1.0;
KMETTCOHC=3.6;
KURNTCAC=0.070; KMETTCAC=0.62;
KBILEC=1.0; KEHRC=0.016; KURNTCOGC=4.7;
KDCVGC=0.23; FRACKIDDCVCC=1.9;
KNATC=0.12; KKIDBIOACTC=0.075;
```

Abbas97a_Mouse.m

```
% Abbas R and Fisher J. 1997. A
physiologically based
%  pharmacokinetic model for
trichloroethylene and its
%  metabolites, chloral hydrate,
trichloroacetate,
%  dichloroacetate, trichloroethanol, and
%  trichloroethanol glucuronide in B6C3F1
mice.
%  Toxicol Appl Pharmacol 147: 15-30.
% Male B6C3F1 mice, 25-30 grams
% Oral dosing of 300, 600, 1200 or 2000
mg/kg TCE in corn
```

```
%  oil (dose volume of 0.5 mL, 20 mL corn
oil/kg BW)

ResetDoses
Mouse
Output=[];

BW=0.0275; PDOSE=1200.0; TCHNG=0.05;
TSTP=193.0; CINT=0.5;
start @NoCallback

Output=addcolsj(Output,_hours,@Justification=
'begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_cbldtca,@Justificatio
n='begin');
Output=addcolsj(Output,_cfat,@Justification='
begin');
Output=addcolsj(Output,_ckid,@Justification='
begin');
Output=addcolsj(Output,_cliv,@Justification='
begin');
Output=addcolsj(Output,_clivtca,@Justificatio
n='begin');
Output=addcolsj(Output,_clivtcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_clivtcoh,@Justificati
on='begin');
Output=addcolsj(Output,_ctcogtcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_ctcoh,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification='
begin');
Output=addcolsj(Output,_zaurntca,@Justificati
on='begin');

PDOSE=2000.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification=
'begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_cbldtca,@Justificatio
n='begin');
Output=addcolsj(Output,_cfat,@Justification='
begin');
Output=addcolsj(Output,_ckid,@Justification='
begin');
Output=addcolsj(Output,_cliv,@Justification='
begin');
Output=addcolsj(Output,_clivtca,@Justificatio
n='begin');
Output=addcolsj(Output,_clivtcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_clivtcoh,@Justificati
on='begin');
Output=addcolsj(Output,_ctcogtcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_ctcoh,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification='
begin');
Output=addcolsj(Output,_zaurntca,@Justificati
on='begin');

PDOSE=300.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification=
'begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_cbldtca,@Justificatio
n='begin');
Output=addcolsj(Output,_cfat,@Justification='
begin');
Output=addcolsj(Output,_ckid,@Justification='
begin');
Output=addcolsj(Output,_cliv,@Justification='
begin');
Output=addcolsj(Output,_clivtca,@Justificatio
n='begin');
Output=addcolsj(Output,_clivtcoh,@Justificati
on='begin');
Output=addcolsj(Output,_ctcogtcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_ctcoh,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification='
begin');
Output=addcolsj(Output,_zaurntca,@Justificati
on='begin');

PDOSE=600.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification=
'begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_cbldtca,@Justificatio
n='begin');
Output=addcolsj(Output,_cfat,@Justification='
begin');
Output=addcolsj(Output,_ckid,@Justification='
begin');
Output=addcolsj(Output,_cliv,@Justification='
begin');
Output=addcolsj(Output,_clivtca,@Justificatio
n='begin');
Output=addcolsj(Output,_clivtcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_clivtcoh,@Justificati
on='begin');
Output=addcolsj(Output,_ctcogtcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_ctcoh,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification='
begin');
Output=addcolsj(Output,_zaurntca,@Justificati
on='begin');

save Output @file='Abbas97a_Mouse_Output.txt'
@format=ascii
```

Abbas97b_Mouse.m

```
% Abbas R, Seckel C, MacMahon K and Fisher
J. 1997.
%  Determination of kinetic rate constants
for chloral
%  hydrate, trichloroethanol,
trichloroacetic acid and
%  dichloroacetic acid: A physiologically
based modeling
%  approach. Toxicologist 36: 32-33.
% B6C3FI mice
% IV dose of 100 mg/kg TCA or TCOH

ResetDoses
Mouse
```

```
Output=[];

BW=0.035; IVDOSETCA=100.0; TCHNG=0.05;
TSTP=170.0; CINT=0.5;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

IVDOSETCA=0.0; IVDOSETCOH=100.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');

save Output
@file='Abbas97b_Mouse_Output.txt'
@format=ascii
```

Fisher91_Mouse.m

```
% Fisher J, Gargas M, Allen B and Andersen
M. 1991.
%  Physiologically based pharmacokinetic
modeling with
%  trichloroethylene and its metabolite,
trichloroacetic
%  acid, in the rat and mouse. Toxicol Appl
Pharmacol 109:
%  183-195.
% B6C3Fl female and male mice
% Open or closed chamber inhalation of
various
%  concentrations of TCE for 4 hours

ResetDoses
Mouse
Output=[];

% Female mice -- inhalation of 42, 236, 368
or 889 ppm TCE
%  for 4 hours
BW=0.025; CONC=42.0; TCHNG=4.0; TSTP=31.0;
CINT=0.01;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.023; CONC=236.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.024; CONC=368.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.03; CONC=889.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

% Female mice -- closed chamber inhalation
of 300, 700,
%  1100, 3700 or 7000 ppm TCE (chamber
volume of 9.1 L)
BW=0.022; CC=1; CONC=1100.0; NRODENTS=14.0;
VCHC=9.1;
KLOSSC=exp(-3.912); TCHNG=4.0; TSTP=4.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

BW=0.024; CONC=300.0; TCHNG=2.0; TSTP=2.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

BW=0.022; CONC=3700.0; TCHNG=6.0; TSTP=6.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

BW=0.021; CONC=700.0; TCHNG=3.0; TSTP=3.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

BW=0.022; CONC=7000.0; TCHNG=6.0; TSTP=6.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

% Male mice -- inhalation of 110, 297, 368
or 748 ppm TCE
%  for 4 hours
CC=0;
BW=0.031; CONC=110.0; TCHNG=4.0; TSTP=25.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

CONC=297.0;
```

```
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

CONC=368.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

CONC=748.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

% Male mice -- closed chamber inhalation of
1020, 1800,
%  3800, 5600 or 10000 ppm TCE (chamber
volume of 9.1 L)
CC=1;
BW=0.026; CONC=1800.0; NRODENTS=15.0;
VCHC=9.1;
KLOSSC=exp(-3.912); TCHNG=3.0; TSTP=3.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

BW=0.03; CONC=1020.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

BW=0.026; CONC=10000.0; TCHNG=4.0; TSTP=4.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

BW=0.03; CONC=3800.0; TCHNG=6.0; TSTP=6.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

BW=0.028; CONC=5600.0; TCHNG=6.0; TSTP=6.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

save Output
@file='Fisher91_Mouse_Output.txt'
@format=ascii
```

Fisher93_Mouse.m

```
% Fisher J and Allen B. 1993. Evaluating the
risk of liver
%  cancer in humans exposed to
trichloroethylene using
%  physiological models. Risk Anal 13: 87-
95.
% Female and male mice
% Oral gavage of various doses of TCE

ResetDoses
Mouse
Output=[];

% Female mice -- oral gavage of 487, 973 or
1947 mg/kg TCE
BW=0.0257; PDOSE=1947.0; TCHNG=0.05;
TSTP=73.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.0273; PDOSE=487.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.0238; PDOSE=973.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

% Male mice -- oral gavage of 487, 973 or
1947 mg/kg TCE
BW=0.0306; PDOSE=1947.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.0338; PDOSE=487.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.0306; PDOSE=973.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
```

```
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
save Output
@file='Fisher93_Mouse_Output.txt'
@format=ascii
```

Green85_Mouse.m

```
% Green T and Prout M. 1985. Species
differences in response
%  to trichloroethylene: II.
Biotransformation in rats and
%  mice.  Toxicol Appl Pharmacol 79: 401-
411.
% Male mice (25 to 32 g) of the B6C3FI and
Swiss-Webster
%  strains (N=4 each/group)
% Oral dosing of 10, 500, 1000 or 2000 mg/kg
containing
%  10 uCi trichloro[1,2-14C]ethylene in corn
oil (0.5 mL to
%  mice)

ResetDoses
Mouse
Output=[];

BW=0.0285; PDOSE=10.0; TCHNG=0.05;
TSTP=73.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_zaexhpost,@Justifica
tion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

PDOSE=1000.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_zaexhpost,@Justifica
tion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

PDOSE=2000.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_zaexhpost,@Justifica
tion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

PDOSE=500.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justifi
cation='begin');
Output=addcolsj(Output,_zaexhpost,@Justifica
tion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

save Output @file='Green85_Mouse_Output.txt'
@format=ascii
```

Greenberg99_Mouse.m

```
% Greenberg M, Burton G and Fisher J. 1999.
Physiologically
%  based pharmacokinetic modeling of inhaled
%  trichloroethylene and its oxidative
metabolites in B6C3F1
%  mice.  Toxicol Appl Pharmacol 154: 264-
278.
% Male B6C3F1 mice, 28-32 grams (N=6/time
point)
% Inhalation of 100 or 600 ppm TCE for 4
hours

ResetDoses
Mouse
Output=[];

BW=0.03; CONC=100.0; TCHNG=4.0; TSTP=50.0;
CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cfat,@Justification=
'begin');
Output=addcolsj(Output,_ckid,@Justification=
'begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');
Output=addcolsj(Output,_clivtca,@Justificati
on='begin');
Output=addcolsj(Output,_clivtcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_clivtcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_ctcogtcoh,@Justifica
tion='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

CONC=600.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cfat,@Justification=
'begin');
Output=addcolsj(Output,_ckid,@Justification=
'begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');
Output=addcolsj(Output,_clivtca,@Justificati
on='begin');
Output=addcolsj(Output,_clivtcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_clivtcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_ctcogtcoh,@Justifica
tion='begin');
```

```
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

save Output
@file='Grnberg99_Mouse_Output.txt'
@format=ascii
```

Larson92a_Mouse.m

```
% Larson J and Bull R. 1992. Species
differences in the
%  metabolism of trichloroethylene to the
carcinogenic
%  metabolites trichloroacetate and
dichloroacetate. Toxicol
%  Appl Pharmacol 115: 278-285.
% Male B6C3Fl mice (26.4 +/- 3.2 grams)
(N=5-6/time point)
% Fasted 4 hr
% Oral dosing of 1.5, 4.5 or 15 mmol TCE/kg
in Tween 80
%  (constant volume of 10 mL/kg to mice)
(197.25, 591.75 and
%  1972.5 mg/kg)

ResetDoses
Mouse
Output=[];

BW=0.0264; PDOSE=197.25; TCHNG=0.05;
TSTP=50.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldmix,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');

PDOSE=1972.5;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldmix,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');

PDOSE=591.75;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldmix,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');

save Output
@file='Larson92a_Mouse_Output.txt'
@format=ascii
```

Larson92b_Mouse.m

```
% Larson J and Bull R. 1992. Metabolism and
lipoperoxidative
%  activity of trichloroacetate and
dichloroacetate in rats
%  and mice. Toxicol Appl Pharmacol 115:
268-277.
% Male B6C3FI mice (27 +/- 2 grams)
% Oral gavage of 5, 20 or 100 mg/kg TCA (5-
20 uCi of
%  [14C]TCA)

ResetDoses
Mouse
Output=[];

BW=0.0264; PODOSETCA=20.0; TCHNG=0.05;
TSTP=25.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');

PODOSETCA=100.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');

save Output
@file='Larson92b_Mouse_Output.txt'
@format=ascii
```

Merdink98_Mouse.m

```
% Merdink J, Gonzalez-Leon A, Bull R and
Schultz I. 1998. The
%  extent of dichloroacetate formation from
%  trichloroethylene, chloral hydrate,
trichloroacetate, and
%    trichloroethanol in B6C3F1 mice.
Toxicol Sci 45: 33-41.
% Male B6C3F1 mice (20–25 grams)
% Fasted 4–8 h prior to dosing
% IV dosing of 100 mg/kg TCE, as a
suspension in 5% Alkamuls,
%  into either an indwelling jugular vein
cannula or a
%  lateral tail vein

ResetDoses
Mouse
Output=[];

BW=0.0225; IVDOSE=100.0; TCHNG=0.05;
TSTP=7.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');

save Output
@file='Merdink98_Mouse_Output.txt'
@format=ascii
```

Prout85_Mouse.m

```
% Prout M, Provan W and Green T. 1985.
Species differences in
%  response to trichloroethylene: I
pharmacokinetics in rats
%  and mice. Toxicol Appl Pharmacol 79:389-
400.
% Male B6C3F1 and Swiss-Webster mice, 25-32
grams (N=4 or 2
%  mice/group
% Oral dosing of 10, 500, 1000 or 2000 mg/kg
%  trichloro[14C]ethylene in corn oil (0.5
mL)(containing
%  10 uCi)

ResetDoses
Mouse
Output=[];

BW=0.0295; PDOSE=1000.0; TCHNG=0.05;
TSTP=45; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldmix,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaexhpost,@Justifica
tion='begin');

save Output @file='Prout85_Mouse_Output.txt'
@format=ascii
```

Templin93_Mouse.m

```
% Templin M, Parker J and Bull R. 1993.
Relative formation of
%  dichloroacetate and trichloroacetate from
%  trichloroethylene in male B6C3F1 mice.
Toxicol Appl
%  Pharmacol 123: 1-8.
% Male B6C3F1 mice, 7 weeks of age (N=4/time
point)
% Oral dosing of 3.8 mmol/kg (499.282 mg/kg)
%  trichloroethylene in 2% polyoxyethylcnc-
sorbitan
%  monooleate (Tween 80)

ResetDoses
Mouse
Output=[];

BW=0.027; PDOSE=500.0; TCHNG=0.05;
TSTP=37.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldmix,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');

save Output
@file='Templin93_Mouse_Output.txt'
@format=ascii
```

APPENDIX F. M FILES FOR RAT SIMULATIONS

The following M files are for generating rat output for validation figures in Appendix B.

Rat.m

```
% Use posterior values
% Remove DCVG compartment

RatPost
FRACKIDDCVCC=exp(10.0); KDCVGC=exp(10.0);
```

RatPrior.m

```
% Parameters from Table A-4 (same as
baselines in model
%  code except for VMaxLungLiv so used value
from model
%  code)
% DRespC, PEffDCVG, kAS, kTSD, kAD, kASTCA,
kASTCOH,
%  FracOtherC, KMClara, FracLungSysC,
VMaxTCOHC, KMTCOH,
%  VMaxGlucC, KMGluc, kMetTCOHC, kMetTCAC,
kBileC, kEHRC,
%  kDCVGC, kNATC, kKidBioactC from Table 3-
38 in report
% kTD from model code (comment from model -
"assume no
%  fecal excretion – 100% absorption")
% kAsTCOH from Table A-12
% FracKidDCVC from model code (comment from
model –
%  "In ".in" files, set to 1, so that all
kidney GSH
%  conjugation is assumed to directly
produce DCVC (model
%  lacks identifiability otherwise)."

SPECIES=2;
BW=0.3; QCC=13.3; VPR=1.9; DRESPC=0.99;
QFATC=0.07; QGUTC=0.153; QKIDC=0.141;
QLIVC=0.021;
QSLWC=0.336;
VBLDC=0.074; VFATC=0.07; VGUTC=0.032;
VKIDC=0.007;
VLIVC=0.034;
VRAPC=0.088; VRESPLUMC=0.004667;
VRESPC=0.0005;
VPERFC=0.8995;
FRACPLAS=0.53;
PB=22.0; PFAT=27.0; PGUT=1.4; PKID=1.3;
PLIV=1.5; PRAP=1.3;
PRESP=1.0; PSLW=0.58;
PRBCPLASTCA=0.5; PBODTCAC=0.88;
PLIVTCAC=1.18;
PBODTCOH=1.11; PLIVTCOH=1.3;
PBODTCOG=1.11; PLIVTCOG=1.3; PEFFDCVG=1.0;
BMAXKDC=1.22; KDISSOC=275.0;
KAS=0.73; KTSD=1.4; KAD=0.96; KTD=0.0;
KASTCA=0.83;
KASTCOH=0.69;
VMAXC=600.0; KMC=21.0; CL=1.0;
FRACTCAC=0.32; FRACOTHERC=0.028;
VMAXDCVGC=66.0; KMDCVGC=1.0; CLDCVG=0.25;
VMAXKIDDCVGC=18.0; KMKIDDCVGC=1.0;
CLKIDDCVG=0.026;
VMAXLUNGLIV=0.0143; KMCLARA=0.016;
FRACLUNGSYSC=4.6;
VMAXTCOHC=1.9; KMTCOH=1.0; CLTCOH=1.0;
VMAXGLUCC=67.0; KMGLUC=31.0; CLGLUC=1.0;
KMETTCOHC=3.1;
KURNTCAC=0.522; KMETTCAC=0.56;
KBILEC=1.0; KEHRC=0.0096; KURNTCOGC=0.522;
KDCVGC=22202.0; FRACKIDDCVCC=1.0;
KNATC=0.11; KKIDBIOACTC=0.09;
```

RatPost.m

```
% Parameters from Table A-4 (same as
baselines in model
%  code except for VMaxLungLiv so used value
from model
%  code) and posterior changes in Table A-12
% Baselines for DRespC, PEffDCVG, kAS, kTSD,
kAD, kASTCA,
%  kASTCOH, FracOtherC, KMClara,
FracLungSysC, VMaxTCOHC,
%  KMTCOH, VMaxGlucC, KMGluc, kMetTCOHC,
kMetTCAC, kBileC,
%  kEHRC, kDCVGC, kNATC, kKidBioactC from
Table 3-38 in
%  report
% Baseline for kTD from model code (comment
from model –
%  "assume no fecal excretion -- 100%
absorption")
% Baseline for kAsTCOH from Table A-12
% Baseline for FracKidDCVC from model code
(comment from
%  model - "In ".in" files, set to 1, so
that all kidney
%  GSH conjugation is assumed to directly
produce DCVC
%  (model lacks identifiability otherwise)."

SPECIES=2;
BW=0.3; QCC=16.0; VPR=1.2; DRESPC=2.765;
QFATC=0.082; QGUTC=0.18; QKIDC=0.14;
QLIVC=0.022;
QSLWC=0.31;
VBLDC=0.074; VFATC=0.068; VGUTC=0.031;
VKIDC=0.007;
VLIVC=0.033;
VRAPC=0.087; VRESPLUMC=0.004672;
VRESPC=0.0005;
VPERFC=0.8995;
FRACPLAS=0.55;
PB=19.0; PFAT=32.0; PGUT=1.1; PKID=1.2;
PLIV=1.6; PRAP=1.3;
PRESP=1.0; PSLW=0.73;
PRBCPLASTCA=0.49; PBODTCAC=1.0;
PLIVTCAC=1.5;
PBODTCOH=1.0; PLIVTCOH=1.2;
PBODTCOG=2.2; PLIVTCOG=10.0; PEFFDCVG=1.0;
BMAXKDC=1.2; KDISSOC=278.0;
KAS=2.5; KTSD=3.7; KAD=0.17; KTD=0.0;
KASTCA=1.5; KASTCOH=0.69;
VMAXC=537.0; KMC=0.50; CL=1.0;
FRACTCAC=0.075; FRACOTHERC=0.34;
```

```
VMAXDCVGC=511.0; KMDCVGC=1.0; CLDCVG=0.089;
VMAXKIDDCVGC=1.3; KMKIDDCVGC=1.0;
CLKIDDCVG=4.8;
VMAXLUNGLIV=0.038; KMCLARA=0.026;
FRACLUNGSYSC=2.7;
VMAXTCOHC=1.8; KMTCOH=22.0; CLTCOH=1.0;
VMAXGLUCC=29.0; KMGLUC=6.6; CLGLUC=1.0;
KMETTCOHC=2.4;
KURNTCAC=0.037; KMETTCAC=0.36;
KBILEC=9.0; KEHRC=1.4; KURNTCOGC=11.0;
KDCVGC=22202.0; FRACKIDDCVCC=1.0;
KNATC=0.00204; KKIDBIOACTC=0.0066;
```

Bernauer96_Rat.m

```
% Bernauer U, Birner G, Dekant W and
Henschler D. 1996.
%  Biotransformation of trichloroethene:
Dose-dependent
%  excretion of 2,2,2-trichloro-metabolites
and mercapturic
%  acids in rats and humans after
inhalation. Arch Toxicol
%  70: 338-346.
http://dx.doi.org/10.1007/s002040050283.
% 2 male Wistar (300-350 g) and 2 female
Wister (200-250 g)
%  exposed simultaneously with humans
% Inhalation of 40, 80 or 160 ppm TCE
stabilized with
%  diisopropylamine (40 ppm) for 6 hours

ResetDoses
Rat
Output=[];

BW=0.325; CONC=40.0; TCHNG=6.0; TSTP=50.0;
CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaurnndcvc,@Justific
ation='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=80.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaurnndcvc,@Justific
ation='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=160.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaurnndcvc,@Justific
ation='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

save Output
@file='Bernauer96_Rat_Output.txt'
@format=ascii
```

Dallas91_Rat.m

```
% Dallas C, Gallo J, Ramanathan R,
Muralidhara S and Bruckner
%  J. 1991.  Physiological pharmacokinetic
modeling of
%  inhaled trichloroethylene in rats.
Toxicol Appl Pharmacol
%  110: 303-314.
% Male SD rats (325-375 g)
% Nose-only inhalation of 50 or 500 ppm TCE
for 2 hours

ResetDoses
Rat
Output=[];

BW=0.35; CONC=50.0; TCHNG=2.0; TSTP=6.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cart,@Justification=
'begin');
Output=addcolsj(Output,_cmixexh,@Justificati
on='begin');

CONC=500.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cart,@Justification=
'begin');
Output=addcolsj(Output,_cmixexh,@Justificati
on='begin');

save Output @file='Dallas91_Rat_Output.txt'
@format=ascii
```

Fisher89_Rat.m

```
% Fisher J, Whittaker T, Taylor D, Clewell H
III and Andersen
%  M. 1989.  Physiologically based
pharmacokinetic modeling
%  of the pregnant rat: A multiroute
exposure model for
%  trichloroethylene and its metabolite,
trichloroacetic
%  acid. Toxicol Appl Pharmacol 99: 395-414.
%    http://dx.doi.org/10.1016/0041-
008X(89)90149-X.
% Female F344 rats
% Closed-chamber inhalation of 300, 1100,
2200 or 5100 ppm
%  TCE

ResetDoses
Rat
Output=[];

CC=1;
BW=0.159; CONC=1100.0; NRODENTS=4.0;
VCHC=9.1;
KLOSSC=exp(-3.912); TCHNG=3.0; TSTP=3.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
```

```
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');
BW=0.159; CONC=2200.0; TCHNG=6.0; TSTP=6.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

BW=0.161; CONC=300.0; TCHNG=2.0; TSTP=2.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

BW=0.175; CONC=5100.0; TCHNG=7.0; TSTP=7.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

save Output @file='Fisher89_Rat_Output.txt'
@format=ascii
```

Fisher91_Rat.m

```
% Fisher J, Gargas M, Allen B and Andersen
M. 1991.
%  Physiologically based pharmacokinetic
modeling with
%  trichloroethylene and its metabolite,
trichloroacetic
%  acid, in the rat and mouse. Toxicol Appl
Pharmacol 109:
%  183-195.
% Female and male Fischer 344 rats
% Inhalation of 600 or 505 ppm TCE for 4
hours

ResetDoses
Rat
Output=[];

BW=0.186; CONC=600.0; TCHNG=4.0; TSTP=50.0;
CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.236; CONC=505.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');

save Output @file='Fisher91_Rat_Output.txt'
@format=ascii
```

Green85_Rat.m

```
% Green T and Prout M. 1985. Species
differences in response
%  to trichloroethylene: II.
Biotransformation in rats and
%  mice. Toxicol Appl Pharmacol 79: 401-411.
%  http://dx.doi.org/10.1016/0041-
008X(85)90138-3.
% Male rats (180 to 200 g) of the Osborne-
Mendel and Alderley
%  Park (Wistar derived) strains
% IV dose of 10 mg/kg Trichloro[2-14C]acetic
acid (12.5 uCi)
%  in water (0.25 mL) injected in tail vein
% OR oral dose of 75 mg/kg Trichloro[2-
14C]acetic acid
%  (9 uCi) in water
% OR oral dose of 500 mg/kg TCE (10 uCi) in
corn oil
%  (5 mL/kg) with or without bile cannulated

ResetDoses
Rat
Outpt=[];

BW=0.19; IVDOSETCA=10.0; TCHNG=0.05;
TSTP=25.0; CINT=0.1;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');

IVDOSETCA=0.0; PODOSETCA=75.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');

PODOSETCA=0.0; PDOSE=500.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntcogtcoh,@Justific
ation='begin');
Outpt=addcolsj(Outpt,_zaurntca,@Justificatio
n='begin');

KEHRC=exp(-100.0);
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_zabiletcog,@Justificat
ion='begin');

save Output @file='Green85_Rat_Output.txt'
@format=ascii
```

Hissink02_Rat.m

```
% Hissink E, Bogaards J, Freidig A,
Commandeur J, Vermeulen N
%  and van Bladeren P. 2002. The use of in
vitro metabolic
%  parameters and physiologically based
pharmacokinetic
%  (PBPK) modeling to explore the risk
assessment of
```

```
% trichloroethylene.  Environ Toxicol
Pharmacol 11:259-271.
% http://dx.doi.org/10.1016/S1382-
6689(02)00019-4.
% Adult male Wistar rats (250-300 g, 9-10
weeks old)
% IV dosing of 10 or 75 mg/kg [1,2-14C]-
trichloroethylene in
% Intralipid† 30% (specific activity: 61.3
or 5.70 KBq/mg)
% OR oral dose of 100 or 1000 mg/kg [1,2-
14C]-
% trichloroethylene in corn oil (specific
activity: 9.22 or
% 0.83 KBq/mg)

ResetDoses
Rat
Outpt=[];

BW=0.275; IVDOSE=10.0; TCHNG=0.05;
TSTP=170.0; CINT=0.5;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_cven,@Justification='b
egin');

IVDOSE=75.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_cven,@Justification='b
egin');

IVDOSE=0.0; PDOSE=100.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_cven,@Justification='b
egin');

PDOSE=1000.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_cven,@Justification='b
egin');

save Output @file='Hissink02_Rat_Output.txt'
@format=ascii
```

Kaneko94_Rat.m

```
% Kaneko T, Wang P-Y and Sato A. 1994.
Enzymes induced by
% ethanol differently affect the
pharmacokinetics of
% trichloroethylene and 1,1,1-
trichloroethane. Occup Environ
% Med 51: 113-119.
% Male Wistar rats, 8 weeks old, put on
study at 10 weeks
% Inhalation of 50, 100, 500 or 1000 ppm TCE
for 6 hours

ResetDoses
Rat
Output=[];

CONC=50.0; TCHNG=6.0; TSTP=50.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=100.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=1000.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=500.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

save Output @file='Kaneko94_Rat_Output.txt'
@format=ascii
```

Keys03_Rat.m

```
% Keys D, Bruckner J, Muralidhara S and
Fisher J. 2003.
% Tissue dosimetry expansion and cross-
validation of rat and
% mouse physiologically based
pharmacokinetic models for
% trichloroethylene. Toxicol Sci 76: 35-50.
% http://dx.doi.org/10.1093/toxsci/kfg212.
% Male SD rats (0.291-0.355 g)
% Intra-arterial dosing of 8 mg/kg TCE in 5%
Alkamuls®
% aqueous emulsion (injected volume of 0.3
ml/animal)
% injected over 30-second period
```

```
% OR inhalation of 50 or 500 ppm TCE for 2
hr
% OR oral dosing of 8 mg TCE/kg TCE in 5%
Alkamuls® (total
%  volume 0.7 to 1.0 ml per rat)

ResetDoses
Rat
Output=[];

BW=0.355; IADOSE=8.0; TCHNG=0.05; TSTP=25.0;
CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cfat,@Justification=
'begin');
Output=addcolsj(Output,_cgut,@Justification=
'begin');
Output=addcolsj(Output,_ckid,@Justification=
'begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');
Output=addcolsj(Output,_cmus,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

IADOSE=0.0;
BW=0.291; CONC=50.0; TCHNG=2.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cfat,@Justification=
'begin');
Output=addcolsj(Output,_cgut,@Justification=
'begin');
Output=addcolsj(Output,_ckid,@Justification=
'begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');
Output=addcolsj(Output,_cmus,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.269; CONC=500.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cfat,@Justification=
'begin');
Output=addcolsj(Output,_cgut,@Justification=
'begin');
Output=addcolsj(Output,_ckid,@Justification=
'begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');
Output=addcolsj(Output,_cmus,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

CONC=0.0;
BW=0.355; PDOSE=8.0; TCHNG=0.05;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cfat,@Justification=
'begin');
Output=addcolsj(Output,_cgut,@Justification=
'begin');
Output=addcolsj(Output,_ckid,@Justification=
'begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');
Output=addcolsj(Output,_cmus,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

save Output @file='Keys03_Rat_Output.txt'
@format=ascii
```

Kimmerle73_Rat.m

```
% Kimmerle G and Eben A. 1973. Metabolism,
excretion and
%  toxicology of trichloroethylene after
inhalation: 1.
%  Experimental exposure on rats.  Arch
Toxicol 30: 115-126.
%  http://dx.doi.org/10.1007/BF02425929.
% Male Wistar rats
% Inhalation of 0, 49, 54, 175, 330 or 3160
ppm TCE for 4 hr

ResetDoses
Rat
Output=[];

BW=0.3; CONC=49.0; TCHNG=4.0; TSTP=77.0;
CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaexhpost,@Justifica
tion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=54.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');

CONC=175.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaexhpost,@Justifica
tion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=330.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaexhpost,@Justifica
tion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');
```

```
CONC=3160.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

save Output
@file='Kimmerle73_Rat_Output.txt'
@format=ascii
```

Larson92a_Rat.m

```
% Larson J and Bull R. 1992. Metabolism and
lipoperoxidative
%  activity of trichloroacetate and
dichloroacetate in rats
%  and mice. Toxicol Appl Pharmacol 115:
268-277.
%  http://dx.doi.org/10.1016/0041-
008X(92)90332-M.
% Male F344 rats (331 +/- 24 g)
% Oral dosing of 20 or 100 mg/kg TCA
following fasting for 24
%  hrs

ResetDoses
Rat
Output=[];

BW=0.331; PODOSETCA=20.0; TCHNG=0.05;
TSTP=33.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');

PODOSETCA=100.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');

save Output @file='Larson92a_Rat_Output.txt'
@format=ascii
```

Larson92b_Rat.m

```
% Larson J and Bull R. 1992. Species
differences in the
%  metabolism of trichloroethylene to the
carcinogenic
%  metabolites trichloroacetate and
dichloroacetate. Toxicol
%  Appl Pharmacol 115: 278-285.
%  http://dx.doi.org/10.1016/0041-
008X(92)90333-N.
% Male Sprague-Dawley rats (404 +/- 91 g)
% Oral dosing of 1.5, 4.5 or 23 mmol TCE/kg
in Tween 80
%  (constant volume of 3 ml/kg) after
fasting for 24 hours

ResetDoses
Rat
Output=[];

BW=0.404; PDOSE=197.25; TCHNG=0.05;
TSTP=50.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

PDOSE=3024.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

PDOSE=591.75;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

save Output @file='Larson92b_Rat_Output.txt'
@format=ascii
```

Lee00_Rat.m

```
% Lee K, Muralidhara S, Schnellmann R and
Bruckner J. 2000.
%  Contribution of direct solvent injury to
the dose-
%  dependent kinetics of trichloroethylene:
Portal vein
%  administration to rats. Toxicol Appl
Pharmacol 164: 46-54.
%  http://dx.doi.org/10.1006/taap.2000.8891.
% Adult male Sprague–Dawley rats (320–380 g
at
%  experimentation)
% Injected dosing of 16 mg TCE/kg BW in 10-
sec IV or PV
%  injection

ResetDoses
Rat
Output=[];

BW=0.275; IVDOSE=16.0; TCHNG=0.0028;
TSTP=0.1; CINT=0.001;
AVGINT=0.01;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldmix,@Justificati
on='begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');
```

```
IVDOSE=0.0; PVDOSE=16.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldmix,@Justificati
on='begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');

save Output @file='Lee00_Rat_Output.txt'
@format=ascii
```

Merdink99_Rat.m

```
% Merdink J, Stenner R, Stevens D, Parker J
and Bull R. 1999.
%  Effect of enterohepatic circulation on
the
%  pharmacokinetics of chloral hydrate and
its metabolites in
%  F344 rats. J Toxicol Environ Health A 57:
357-368.
%
http://dx.doi.org/10.1080/009841099157665.
% Male Fischer 344 rats (250–300 g)
% IV dosing of 100 mg/kg TCOH

ResetDoses
Rat
Output=[];

BW=0.275; IVDOSETCOH=100.0; TCHNG=3.0;
TSTP=9.0; CINT=0.05;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
save Output @file='Merdink99_Rat_Output.txt'
@format=ascii
```

Prout85_Rat.m

```
% Prout M, Provan W and Green T. 1985.
Species differences in
%  response to trichloroethylene: I
pharmacokinetics in rats
%  and mice. Toxicol Appl Pharmacol 79: 389-
400.
% Male Alderley Park Wistar OR Osborne-
Mendel derived rats,
%  180-200g
% Oral dosing of 10, 500, 1000 or 2000 mg/kg
%  trichloro[14C]ethylene (10 uCi) in corn
oil

ResetDoses
Rat
Outpt=[];

% Non-specified rats
BW=0.19; PDOSE=1000.0; TCHNG=0.05;
TSTP=41.0; CINT=0.1;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_cart,@Justification='b
egin');
Outpt=addcolsj(Outpt,_cbldtca,@Justification
='begin');
Outpt=addcolsj(Outpt,_ctcoh,@Justification='
begin');
Outpt=addcolsj(Outpt,_zaexhpost,@Justificati
on='begin');

% Alderley Park Wistar rats
PDOSE=10.0; TSTP=73.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_zaexhpost,@Justificati
on='begin');

PDOSE=1000.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_zaexhpost,@Justificati
on='begin');

PDOSE=500.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_zaexhpost,@Justificati
on='begin');

% Osborne-Mendel rats
PDOSE=10.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_zaexhpost,@Justificati
on='begin');


PDOSE=1000.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_zaexhpost,@Justificati
on='begin');

PDOSE=2000.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_zaexhpost,@Justificati
on='begin');

PDOSE=500.0;
start @NoCallback
Outpt=addcolsj(Outpt,_hours,@Justification='
begin');
Outpt=addcolsj(Outpt,_aurntctot_mole,@Justif
ication='begin');
Outpt=addcolsj(Outpt,_zaexhpost,@Justificati
on='begin');

save Output @file='Prout85_Rat_Output.txt'
@format=ascii
```

Simmons02_Rat.m

```
% Simmons J, Boyes W, Bushnell P, Raymer J,
Limsakun T,
%  McDonald A, Sey Y and Evans M. 2002. A
physiologically
%  based pharmacokinetic model for
trichloroethylene in the
%  male Long-Evans rat. Toxicol Sci 69: 3-
15.
%  http://dx.doi.org/10.1093/toxsci/69.1.3.
% Male LE rats (received at ages 60, 65, 90
(+/-2) days)
% Open chamber inhalation of 200, 2000 or
4000 ppm TCE for
%  1 hour
% OR closed chamber inhalation of 100 ppm
TCE for 4 hours or
%  500, 1000 or 3000 ppm TCE for 6 hours

ResetDoses
Rat
Output=[];

% Open chamber
BW=0.42014; VFATC=0.0917; CONC=2000.0;
TCHNG=1.0; TSTP=5.0;
CINT=0.05;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cfat,@Justification=
'begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.40651; VFATC=0.0875; CONC=4000.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cfat,@Justification=
'begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

BW=0.3978625; VFATC=0.08125; CONC=200.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cfat,@Justification=
'begin');
Output=addcolsj(Output,_cliv,@Justification=
'begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

% Closed chamber
Rat
CC=1;
BW=0.408907143; CONC=108.0; NRODENTS=1.0;
VCHC=10.4;
KLOSSC=exp(-3.912); TCHNG=5.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

CONC=864.0; TCHNG=6.0; TSTP=6.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

CONC=2940.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

CONC=506.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cinhppm,@Justificati
on='begin');

save Output @file='Simmons02_Rat_Output.txt'
@format=ascii
```

Stenner97_Rat.m

```
% Stenner R, Merdink J, Stevens D, Springer
D and Bull R.
%  1997. Enterohepatic recirculation of
trichloroethanol
%  glucuronide as a significant source of
trichloroacetic
%  acid. Metabolites of trichloroethylene.
Drug Metab
%  Dispos 25: 529-535.
% Male F-344 rats (~300 g)
% Intraduodenal dosing (via duodenal
cannula) of 100 mg/kg
%  TCE -- modeled as an oral dose
% OR IV dosing of 100 mg/kg of TCOH  without
bile cannulated
% OR IV dosing of 5, 20 or 100 mg/kg of TCOH
with bile
%  cannulated

ResetDoses
Rat
Output=[];

% TCE dosing
BW=0.3; PDOSE=100.0; TCHNG=0.05; TSTP=50.0;
CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcog,@Justification
='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');

% TCOH dosing without bile cannulated
PDOSE=0.0; IVDOSETCOH=100.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
```

```
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% TCOH dosing with bile cannulated
KEHRC=exp(-100.0); IVDOSETCOH=5.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

IVDOSETCOH=20.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

IVDOSETCOH=100.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

save Output @file='Stenner97_Rat_Output.txt'
@format=ascii
```

Templin95_Rat.m

```
% Templin M, Stevens D, Stenner R, Bonate P,
Tuman D and Bull
%  R. 1995.  Factors affecting species
differences in the
%  kinetics of metabolites of
trichloroethylene. J Toxicol
%  Environ Health 44: 435-447.
% Male F344 rats (250-300 g)
% Oral dosing of 0.15 or 0.76 mmol/kg TCE in
2%
%  polyoxyethylene-sorbitan monooleate
(Tween 80)

ResetDoses
Rat
Output=[];

BW=0.275; PDOSE=100.0; TCHNG=0.05;
TSTP=50.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');

save Output @file='Templin95_Rat_Output.txt'
@format=ascii
```

Yu00_Rat.m

```
% Yu K, Barton H, Mahle D and Frazier J.
2000. In vivo
%  kinetics of trichloroacetate in male
Fischer 344 rats.
%  Toxicol Sci 54: 302-311.
% Male Fischer 344 rats (195–235 g)
% IV dosing of 6.1, 61 or 306 mmol/mL TCA
([1-14C] TCA mixed
%  with unlabeled TCA) in physiologic saline
(6–8 uCi of 14C
%  per rat)

ResetDoses
Rat
Output=[];

BW=0.215; IVDOSETCA=1.0; TCHNG=0.05;
TSTP=25.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_clivtca,@Justificati
on='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

IVDOSETCA=10.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_clivtca,@Justificati
on='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

IVDOSETCA=50.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_clivtca,@Justificati
on='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

save Output @file='Yu00_Rat_Output.txt'
@format=ascii
```

APPENDIX G. M FILES FOR HUMAN SIMULATIONS

The following M files are for generating human output for validation figures in Appendix C.

Please note that some lines in this appendix carry over to a second line only because they were too long for WORD. These lines are not too long for acslX in an actual M file and do not include continuation characters; therefore, the break in the lines will need to be removed for using this text in a M file.

Human.m

```
% Use posterior values
% All kidney GSH conjugation is locally
processed

HumanPost
FRACKIDDCVCC=exp(10.0);
```

HumanPrior.m

```
% Parameters from Table A-4 (same as
baselines in model code
%  except for QKidC, FracPlas and
VMaxLungLiv so used value
%  from model code)
% DRespC, PEffDCVG, kAS, kTSD, kAD, kASTCA,
kASTCOH,
%  FracOtherC, KMClara, FracLungSysC,
KMTCOH, ClTCOH, KMGluc,
%  ClGluc, kMetTCOHC, kMetTCAC, kBileC,
kEHRC, kDCVGC, kNATC,
%  kKidBioactC from Table 3-39 in report
% kTD from model code (comment from model -
"assume no fecal
%  excretion – 100% absorption")
% FracKidDCVC from model code (comment from
model – "In ".in"
%  files, set to 1, so that all kidney GSH
conjugation is
%  assumed to directly produce DCVC (model
lacks
%  identifiability otherwise)."

SPECIES=1;
BW=70.0; QCC=16.0; VPR=0.96; DRESPC=1.47;
QFATC=0.05; QGUTC=0.19; QKIDC=0.19;
QLIVC=0.065; QSLWC=0.22;
VBLDC=0.077; VFATC=0.199; VGUTC=0.02;
VKIDC=0.0043;
VLIVC=0.025;
VRAPC=0.088; VRESPLUMC=0.002386;
VRESPC=0.00018;
VPERFC=0.856;
FRACPLAS=0.567;
PB=9.5; PFAT=67.0; PGUT=2.6; PKID=1.6;
PLIV=4.1; PRAP=2.6;
PRESP=1.3; PSLW=2.1;
PRBCPLASTCA=0.5; PBODTCAC=0.52;
PLIVTCAC=0.66;
PBODTCOH=0.91; PLIVTCOH=0.59;
PBODTCOG=0.91; PLIVTCOG=0.59; PEFFDCVG=1.24;
BMAXKDC=4.62; KDISSOC=182.0;
KAS=1.4; KTSD=1.4; KAD=0.75; KTD=0.0;
KASTCA=0.58; KASTCOH=0.49;
VMAXC=255.0; KMC=1.0; CL=66.0;
FRACTCAC=0.32;
FRACOTHERC=0.14;
VMAXDCVGC=1.0; KMDCVGC=2.9; CLDCVG=19.0;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=2.7;
CLKIDDCVG=230.0;
VMAXLUNGLIV=0.0253; KMCLARA=0.019;
FRACLUNGSYSC=3.0;
VMAXTCOHC=1.0; KMTCOH=5.0; CLTCOH=0.35;
VMAXGLUCC=1.0; KMGLUC=10.0; CLGLUC=3.0;
KMETTCOHC=2.47;
KURNTCAC=0.108; KMETTCAC=0.55;
KBILEC=3.47; KEHRC=0.21; KURNTCOGC=0.108;
KDCVGC=0.127; FRACKIDDCVCC=1.0;
KNATC=0.0025; KKIDBIOACTC=0.0064;
```

HumanPost.m

```
% Parameters from Table A-4 (same as
baselines in model code
%  except for QKidC, FracPlas and
VMaxLungLiv so used value
%  from model code) and posterior changes in
Table A-15
% Baselines for DRespC, PEffDCVG, kAS, kTSD,
kAD, kASTCA,
%  kASTCOH, FracOtherC, KMClara,
FracLungSysC, KMTCOH,
%  ClTCOH, KMGluc, ClGluc, kMetTCOHC,
kMetTCAC, kBileC,
%  kEHRC, kDCVGC, kNATC, kKidBioactC from
Table 3-39 in
%  report
% Baseline for kTD from model code (comment
from model –
%  "assume no fecal excretion -- 100%
absorption")
% Baseline for FracKidDCVC from model code
(comment from
%  model - "In ".in" files, set to 1, so
that all kidney GSH
%  conjugation is assumed to directly
produce DCVC (model
%  lacks identifiability otherwise)."

SPECIES=1;
BW=70.0; QCC=13.4; VPR=1.46; DRESPC=0.63;
QFATC=0.04; QGUTC=0.15; QKIDC=0.191;
QLIVC=0.033; QSLWC=0.16;
VBLDC=0.078; VFATC=0.16; VGUTC=0.02;
VKIDC=0.0043;
VLIVC=0.026;
VRAPC=0.088; VRESPLUMC=0.0024;
VRESPC=0.00018; VPERFC=0.856;
FRACPLAS=0.57;
PB=9.2; PFAT=57.0; PGUT=2.8; PKID=1.6;
PLIV=4.1; PRAP=2.4;
PRESP=1.3; PSLW=2.4;
```

```
PRBCPLASTCA=0.20; PBODTCAC=0.62;
PLIVTCAC=0.79;
PBODTCOH=1.5; PLIVTCOH=0.63;
PBODTCOG=0.66; PLIVTCOG=3.9;
PEFFDCVG=0.01007;
BMAXKDC=4.1; KDISSOC=181.0;
KAS=1.4; KTSD=1.4; KAD=0.75; KTD=0.0;
KASTCA=4.5; KASTCOH=8.3;
VMAXC=96.0; KMC=1.0; CL=834.0;
FRACTCAC=0.042; FRACOTHERC=0.12;
VMAXDCVGC=1.0; KMDCVGC=3.5; CLDCVG=53.0;
VMAXKIDDCVGC=1.0; KMKIDDCVGC=0.76;
CLKIDDCVG=10.4;
VMAXLUNGLIV=0.095; KMCLARA=0.27;
FRACLUNGSYSC=24.0;
VMAXTCOHC=1.0; KMTCOH=2.2; CLTCOH=0.18;
VMAXGLUCC=1.0; KMGLUC=133.0; CLGLUC=0.28;
KMETTCOHC=0.75;
KURNTCAC=0.0049; KMETTCAC=0.28;
KBILEC=6.86; KEHRC=0.16; KURNTCOGC=1.7;
KDCVGC=7.12; FRACKIDDCVCC=1.0;
KNATC=0.00032; KKIDBIOACTC=0.065;
```

FemalePrior.m

```
% Parameters from Table A-4 (same as
baselines in model code
%  except for QKidC and VMaxLungLiv so used
value from model
%  code)

BW=60.0;
QFATC=0.085; QGUTC=0.21; QKIDC=0.17;
QSLWC=0.17;
VBLDC=0.068; VFATC=0.317; VGUTC=0.022;
VKIDC=0.0046;
VLIVC=0.023;
VRAPC=0.093; VPERFC=0.85778;
VMAXLUNGLIV=0.0273;
```

FemalePost.m

```
% Parameters from Table A-4 (same as
baselines in model code
%  except for QKidC and VMaxLungLiv so used
value from model
%  code) and posterior changes in Table A-15

BW=60.0;
QFATC=0.066; QGUTC=0.17; QKIDC=0.171;
QSLWC=0.12;
VBLDC=0.069; VFATC=0.25; VGUTC=0.022;
VKIDC=0.0046;
VLIVC=0.024;
VRAPC=0.093; VPERFC=0.85778;
VMAXLUNGLIV=0.103;
```

MalePrior.m

```
% Parameters from Table A-4 (same as
baselines in model code
%  except for QKidC and VMaxLungLiv so used
value from model
%  code)

BW=70.0;
QFATC=0.05; QGUTC=0.19; QKIDC=0.19;
QSLWC=0.22;
VBLDC=0.077; VFATC=0.199; VGUTC=0.02;
VKIDC=0.0043;
VLIVC=0.025;
VRAPC=0.088; VPERFC=0.856;
VMAXLUNGLIV=0.0253;
```

MalePost.m

```
% Parameters from Table A-4 (same as
baselines in model code
%  except for QKidC and VMaxLungLiv so used
value from model
%  code) and posterior changes in Table A-15

BW=70.0;
QFATC=0.04; QGUTC=0.15; QKIDC=0.191;
QSLWC=0.16;
VBLDC=0.078; VFATC=0.16; VGUTC=0.02;
VKIDC=0.0043;
VLIVC=0.026;
VRAPC=0.088; VPERFC=0.856;
VMAXLUNGLIV=0.095;
```

Bernauer96_Human.m

```
% Bernauer U, Birner G, Dekant W and
Henschler D. 1996.
%  Biotransformation of trichloroethene:
Dose-dependent
%  excretion of 2,2,2-trichloro-metabolites
and mercapturic
%  acids in rats and humans after
inhalation. Arch Toxicol
%  70: 338-346.
http://dx.doi.org/10.1007/s002040050283.
% 3 male volunteers, 37-69 years old
% Inhalation of 40, 80 or 160 ppm TCE
stabilized with
%  diisopropylamine (40 ppm) for 6 hours
% Revised for consistency with molar data,
and for
%  1,1+1,2 isomers for DCVC

ResetDoses
Human
MalePost
Output=[];

CONC=40.0; TCHNG=6.0; TSTP=48.0; CINT=0.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaurnndcvc,@Justific
ation='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=80.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaurnndcvc,@Justific
ation='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=160.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
```

```
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_zaurnndcvc,@Justific
ation='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

save Output
@file='Bernauer96_Human_Output.txt'
@format=ascii
```

Chiu07_Human.m

```
% Chiu W, Micallef S, Monster A and Bois F.
2007.
%  Toxicokinetics of inhaled
trichloroethylene and
%  tetrachloroethylene in humans at 1 ppm:
Empirical results
%  and comparisons with previous studies.
Toxicol Sci 95:
%  23-36.
http://dx.doi.org/10.1093/toxsci/kfl129.
% 7 adult male volunteers
% Inhalation dosing of 1 ppm TCE for 6 hours

% Lines setting different inhalation
concentrations were
%  truncated so the values that were there
are used and the
%  average of the values there were used for
the remaining
%  time of exposure

ResetDoses
Human
MalePost
Output=[];

% Experiment A-TRI -- measured QP of 310.8
BW=70.5; VFATC=0.11; QCC=8.796393001;
TCHNG=6.0; CINT=0.5;
AVGINT=0.01;
ConcList=[1.155 1.185 1.322 1.262 1.357
1.282 1.339 1.330
   1.284 1.248 1.077 1.257 1.18
1.252153846];
TStpList=[0.283 0.617 1.117 1.367 1.867
2.117 2.367 2.783
   2.950 3.700 4.117 4.533 4.950 122.0];
CONC=ConcList(1);
TSTP = TStpList(1);
start @NoCallback

for iter = [2 : 14]
    CONC=ConcList(iter);
    TSTP = TStpList(iter);
    continue @NoCallback
end

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

ConcList=[1.019 0.932 1.085 1.031 1.035
1.165 1.238 1.194
   1.200 1.171 1.249 1.194 1.14
1.127153846];
TStpList=[0.300 0.717 1.050 1.383 1.717
2.050 2.383 2.633
   3.050 3.383 3.800 4.300 4.467 142.5];
CONC=ConcList(1);
TSTP = TStpList(1);
start @NoCallback

for iter = [2 : 14]
    CONC=ConcList(iter);
    TSTP = TStpList(iter);
    continue @NoCallback
end

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Experiment B-TRI -- measured QP of 319.2
BW=75.6; VFATC=0.204; QCC=9.034133353;
ConcList=[1.117 1.080 1.107 1.060 1.011
1.067 1.114 1.142
   1.153 1.116 1.133 1.122 1.19
1.108615385];
TStpList=[0.150 0.317 0.983 1.150 1.483
1.733 2.233 2.483
   2.900 3.150 3.400 3.567 3.900 116.5];
CONC=ConcList(1);
TSTP = TStpList(1);
start @NoCallback

for iter = [2 : 14]
    CONC=ConcList(iter);
    TSTP = TStpList(iter);
    continue @NoCallback
end

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
```

```
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');

ConcList=[1.424 1.305 1.367 1.341 1.353
0.492 0.248 0.302
   1.594 1.876 1.642 1.583 1.46
1.229769231];
TStpList=[0.133 0.300 0.467 0.717 1.050
1.300 1.383 1.550
   1.633 1.717 1.800 1.883 1.967 145.0];
CONC=ConcList(1);
TSTP = TStpList(1);
start @NoCallback

for iter = [2 : 14]
    CONC=ConcList(iter);
    TSTP = TStpList(iter);
    continue @NoCallback
end

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');

% Experiment C-TRI -- measured QP of 310.8
BW=75.2; VFATC=0.204; QCC=8.796393001;
ConcList=[1.218 1.155 1.185 1.322 1.262
1.357 1.282 1.339
   1.330 1.284 1.248 1.077 1.25
1.254538462];
TStpList=[0.050 0.550 0.883 1.383 1.633
2.133 2.383 2.633
   3.050 3.217 3.967 4.383 4.800 141.0];
CONC=ConcList(1);
TSTP = TStpList(1);
start @NoCallback

for iter = [2 : 14]
    CONC=ConcList(iter);
    TSTP = TStpList(iter);
    continue @NoCallback
end

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

ConcList=[0.965 1.019 0.932 1.085 1.031
1.035 1.165 1.238
   1.194 1.200 1.171 1.249 1.19
1.113384615];
TStpList=[0.133 0.467 0.883 1.217 1.550
1.883 2.217 2.550
   2.800 3.217 3.550 3.967 4.467 142.0];
CONC=ConcList(1);
TSTP = TStpList(1);
start @NoCallback

for iter = [2 : 14]
    CONC=ConcList(iter);
    TSTP = TStpList(iter);
    continue @NoCallback
end

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Experiment D-TRI-1 -- measured QP of 298.2
BW=70.5; VFATC=0.129; QCC=8.439782474;
ConcList=[1.080 1.117 1.080 1.107 1.060
1.011 1.067 1.114
   1.142 1.153 1.116 1.133 1.12 1.1];
TStpList=[0.050 0.550 0.717 1.383 1.550
1.883 2.133 2.633
   2.883 3.300 3.550 3.800 3.967 132.0];
CONC=ConcList(1);
TSTP = TStpList(1);
start @NoCallback

for iter = [2 : 14]
    CONC=ConcList(iter);
    TSTP = TStpList(iter);
    continue @NoCallback
end

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');
```

```
% Experiment F-TRI -- measured QP of 327.6
BW=69.5; VFATC=0.18; QCC=9.271873704;
ConcList=[1.308 1.218 1.155 1.185 1.322
1.262 1.357 1.282
   1.339 1.330 1.284 1.248 1.07
1.258461538];
TStpList=[0.083 0.333 0.833 1.167 1.667
1.917 2.417 2.667
   2.917 3.333 3.500 4.250 4.667 143.0];
CONC=ConcList(1);
TSTP = TStpList(1);
start @NoCallback
for iter = [2 : 14]
    CONC=ConcList(iter);
    TSTP = TStpList(iter);
    continue @NoCallback
end

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

ConcList=[1.344 1.252 1.424 1.305 1.367
1.341 1.353 0.492
   0.248 0.302 1.594 1.876 1.64
1.195230769];
TStpList=[0.300 0.383 0.633 0.800 0.967
1.217 1.550 1.800
   1.883 2.050 2.133 2.217 2.300 146.0];
CONC=ConcList(1);
TSTP = TStpList(1);
start @NoCallback

for iter = [2 : 14]
    CONC=ConcList(iter);
    TSTP = TStpList(iter);
    continue @NoCallback
end

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Experiment G-TRI-2 -- measured QP of 302.4
BW=71.0; VFATC=0.096; QCC=8.55865265;
ConcList=[1.344 1.252 1.424 1.305 1.367
1.341 1.353 0.492
   0.248 0.302 1.594 1.876 1.64
1.195230769];
TStpList=[0.050 0.133 0.383 0.550 0.717
0.967 1.300 1.550
   1.633 1.800 1.883 1.967 2.050 144.0];
CONC=ConcList(1);
TSTP = TStpList(1);
start @NoCallback


for iter = [2 : 14]
    CONC=ConcList(iter);
    TSTP = TStpList(iter);
    continue @NoCallback
end

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

save Output @file='Chiu07_Human_Output.txt'
@format=ascii
```

Fisher98_Human.m

```
% Fisher J, Mahle D and Abbas R. 1998. A
human
%  physiologically based pharmacokinetic
model for
%  trichloroethylene and its metabolites,
trichloroacetic
%  acid and free trichloroethanol. Toxicol
Appl Pharmacol
%  152: 339-359.
http://dx.doi.org/10.1006/taap.1998.8486.
% Male and female voluteers, 20-36 years old
% Inhalation dosing of 50 or 100 ppm TCE for
4 hours

ResetDoses
Human
MalePost
Output=[];

% Male subject 1
BW=71.4; VFATC=0.17; PB=11.49; CONC=105.5;
TCHNG=4.0;
TSTP=265.0; CINT=0.5;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
```

```
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Male subject 2
BW=69.3; VFATC=0.27; PB=10.1; CONC=49.3;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Male subject 3
BW=71.1; VFATC=0.14; PB=11.1; CONC=55.2;
start @NoCallback

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=101.5;
start @NoCallback

Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Male subject 4
BW=52.3; VFATC=0.1; PB=12.1; CONC=53.1;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=97.8;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Male subject 5
BW=82.3; VFATC=0.14; PB=11.91; CONC=105.5;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Male subject 6
BW=82.7; VFATC=0.14; PB=10.85; CONC=102.6;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
```

```
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Male subject 7
BW=73.2; VFATC=0.18; PB=10.47; CONC=102.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Male subject 8
% PB wasn't set so reset to PB from
HumanPost.m
BW=60.9; VFATC=0.1; CONC=101.1;
PB=9.2;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Male subject 9
% PB wasn't set so reset to PB from
HumanPost.m
BW=70.9; VFATC=0.18; CONC=103.4;
PB=9.2;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

ResetDoses
Human
FemalePost

% Female subject 1
BW=66.5; VFATC=0.32; PB=9.88; CONC=55.1;
TCHNG=4.0;
TSTP=265.0; CINT=0.5;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=101.4;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');
% Female subject 2
BW=62.3; VFATC=0.24; PB=9.45; CONC=53.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

CONC=97.7;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
```

```
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Female subject 3
BW=57.5; VFATC=0.21; PB=6.47; CONC=102.5;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Female subject 4
BW=55.5; VFATC=0.23; PB=7.63; CONC=102.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Female subject 5
BW=67.3; VFATC=0.35; PB=11.0; CONC=102.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Female subject 6
% PB wasn't set so reset to PB from
HumanPost.m
BW=63.2; VFATC=0.26; CONC=101.0;
PB=9.2;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Female subject 7
% PB wasn't set so reset to PB from
HumanPost.m
BW=48.6; VFATC=0.23; CONC=103.3;
PB=9.2;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Female subject 8
BW=61.8; VFATC=0.33; PB=10.37; CONC=102.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cdcvg_mole,@Justific
ation='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
```

```
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

save Output
@file='Fisher98_Human_Output.txt'
@format=ascii
```

Kimmerle73_Human.m

```
% Kimmerle G and Eben A. 1973. Metabolism,
excretion and
%  toxicology of trichloroethylene after
inhalation: 2.
%  Experimental human exposure. Arch Toxicol
30: 127-138.
%  http://dx.doi.org/10.1007/BF02425930.
% Male and female subjects, age 20-50 yrs
(total of 4
%  subjects)
% Single inhalation dosing of 40 or 44 ppm
TCE (+/- 4 ppm)
%  over 4 hours
% OR repeated inahaltion dosing of 48 ppm
TCE (+/- 3 ppm)
%  over 4 hours/day for 5 days

ResetDoses
Human
FemalePost
Out=[];

CONC=40.0; TCHNG=4.0; TSTP=450.0; CINT=0.5;
URNMISSING=1; COLLECTTM=168.0;
COLLECTINT=24.0;
start @NoCallback
Out=addcolsj(Out,_hours,@Justification='begi
n');
Out=addcolsj(Out,_aurntcogtcoh,@Justificatio
n='begin');
Out=addcolsj(Out,_aurntcogtcoh_coll,@Justifi
cation='begin');
Out=addcolsj(Out,_ctcoh,@Justification='begi
n');
Out=addcolsj(Out,_cven,@Justification='begin
');
Out=addcolsj(Out,_zaurntca,@Justification='b
egin');
Out=addcolsj(Out,_zaurntca_coll,@Justificati
on='begin');

CONC=44.0;
start @NoCallback
Out=addcolsj(Out,_hours,@Justification='begi
n');
Out=addcolsj(Out,_aurntcogtcoh,@Justificatio
n='begin');
Out=addcolsj(Out,_aurntcogtcoh_coll,@Justifi
cation='begin');
Out=addcolsj(Out,_ctcoh,@Justification='begi
n');
Out=addcolsj(Out,_cven,@Justification='begin
');
Out=addcolsj(Out,_zaurntca,@Justification='b
egin');
Out=addcolsj(Out,_zaurntca_coll,@Justificati
on='begin');

Human
MalePost
CONC=40.0;
start @NoCallback
Out=addcolsj(Out,_hours,@Justification='begi
n');
Out=addcolsj(Out,_aurntcogtcoh,@Justificatio
n='begin');
Out=addcolsj(Out,_aurntcogtcoh_coll,@Justifi
cation='begin');
Out=addcolsj(Out,_ctcoh,@Justification='begi
n');
Out=addcolsj(Out,_cven,@Justification='begin
');
Out=addcolsj(Out,_zaurntca,@Justification='b
egin');
Out=addcolsj(Out,_zaurntca_coll,@Justificati
on='begin');

CONC=44.0;
start @NoCallback
Out=addcolsj(Out,_hours,@Justification='begi
n');
Out=addcolsj(Out,_aurntcogtcoh,@Justificatio
n='begin');
Out=addcolsj(Out,_aurntcogtcoh_coll,@Justifi
cation='begin');
Out=addcolsj(Out,_ctcoh,@Justification='begi
n');
Out=addcolsj(Out,_cven,@Justification='begin
');
Out=addcolsj(Out,_zaurntca,@Justification='b
egin');
Out=addcolsj(Out,_zaurntca_coll,@Justificati
on='begin');

% Repeated dosing
Human
CONC=48.0; DAYS=5.0; TMAX=100.0;
DOSEINT=24.0;
URNMISSING=1; COLLECTTM=384.0;
COLLECTINT=24.0;
start @NoCallback
Out=addcolsj(Out,_hours,@Justification='begi
n');
Out=addcolsj(Out,_aurntcogtcoh,@Justificatio
n='begin');
Out=addcolsj(Out,_aurntcogtcoh_coll,@Justifi
cation='begin');
Out=addcolsj(Out,_ctcoh,@Justification='begi
n');
Out=addcolsj(Out,_cven,@Justification='begin
');
Out=addcolsj(Out,_zaurntca,@Justification='b
egin');
Out=addcolsj(Out,_zaurntca_coll,@Justificati
on='begin');

save Output
@file='Kimmerle73_Human_Output.txt'
@format=ascii
```

Monster76_Human.m

```
% Monster A, Boersma G and Duba W. 1976.
Pharmacokinetics of
%  trichloroethylene in volunteers,
influence of workload and
%  exposure concentration. Int Arch Occup
Environ Health 38:
%  87-102.
http://dx.doi.org/10.1007/BF00378619.
% Four male volunteers
% Inhalation dosing of 70 or 140 ppm TCE for
4 hours
```

```
ResetDoses
Human
MalePost
Output=[];

% Subject 1 -- measured QP of 210.0
BW=70.0; VFATC=0.12; QCC=5.943508785;
CONC=65.0; TCHNG=4.0;
TSTP=505.0; CINT=0.5;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_retdose,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% measured QP of 282.0
QCC=7.981283225; CONC=140.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_retdose,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Subject 2 -- measured QP of 390.0
BW=80.0; VFATC=0.26; QCC=11.03794489;
CONC=68.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_retdose,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% measured QP of 372.0
QCC=10.52850128; CONC=138.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_retdose,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Subject 3 -- measured QP of 258.0
BW=62.0; VFATC=0.14; QCC=7.302025078;
CONC=70.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_retdose,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% measured QP of 336.0
QCC=9.509614055; CONC=142.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_retdose,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% Subject 4 -- measured QP of 444.0
BW=67.0; VFATC=0.09; QCC=12.56627572;
CONC=76.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
```

```
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_retdose,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

% measured QP of 486.0
QCC=13.75497747; CONC=140.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_calvppm,@Justificati
on='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cven,@Justification=
'begin');
Output=addcolsj(Output,_retdose,@Justificati
on='begin');
Output=addcolsj(Output,_totctcoh,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

save Output
@file='Monster76_Human_Output.txt'
@format=ascii
```

Muller74_Human.m

```
% Muller G, Spassovski M and Henschler D.
1974. Metabolism of
%  trichloroethylene in man: II.
Pharmacokinetics of
%  metabolites. Arch Toxicol 32: 283-295.
%  http://dx.doi.org/10.1007/BF00330110.
% Male students, 20 to 30 years
% Oral dosing with 3 mg/kg NaTCA or 10 mg/kg
TCOH drunk over
%  0.01 hours (36 seconds) (3 mg/kg NaTCA is
equivalent to
%  2.646 mg/kg TCA (NaTCA MW = 185.4 and 1
mg NaTCA equiv to
%  0.8819 mg TCA))

ResetDoses
Human
MalePost
Output=[];

PODOSETCA=2.646; TCHNG=0.01; TSTP=170.0;
CINT=0.5;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

PODOSETCA=0.0; PODOSETCOH=10.0;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_aurntcogtcoh,@Justif
ication='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_ctcoh,@Justification
='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

save Output
@file='Muller74_Human_Output.txt'
@format=ascii
```

Paykoc45_Human.m

```
% Paykoc Z and Powell J. 1945. The excretion
of sodium
%  trichloroacetate.  J Pharmacol Exp Ther
85: 289-293.
% 6 subjects
% IV dosing with 1.7, 1.8 or 2.9 g sodium
trichloroacetate in
%  3% aqueous solution (approximately
isotonic) given over
%  1 hour (BWs of 45.6, 48.2 or 64.0 kg so
doses of 0.03728,
%  0.06016 or 0.028125 g sodium TCA/kg which
convert to 37.2,
%  60.16 or 28.125 mg NaTCA/kg and to 32.9,
53.06 or
%  24.80 mg TCA/kg (NaTCA MW = 185.4, 1 mg
NaTCA equiv to
%  0.8819 mg TCA)

ResetDoses
Human
Output=[];

BW=45.6; FRACPLAS=0.61; IVDOSETCA=32.9;
TCHNG=1.0;
TSTP=203.0; CINT=0.5;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

BW=48.2; FRACPLAS=0.60; IVDOSETCA=53.06;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
Output=addcolsj(Output,_zaurntca,@Justificat
ion='begin');

BW=64.0; FRACPLAS=0.55; IVDOSETCA=24.8;
start @NoCallback
Output=addcolsj(Output,_hours,@Justification
='begin');
Output=addcolsj(Output,_cbldtca,@Justificati
on='begin');
Output=addcolsj(Output,_cplastca,@Justificat
ion='begin');
```

```
save Output
@file='Paykoc45_Human_Output.txt'
@format=ascii
```

APPENDIX H. DATA FOR MOUSE VALIDATION FIGURES

The following data are for generating mouse validation figures in Appendix A.

Abbas and Fisher, 1997a

TCE Oral Gavage 300.0 mg/kg

Hours	AUrnTCOGTCOH	CBldTCA	CFat	CKid	CLiv	CLivTCA	CLivTCOH	CTCOGTCOH	CTCOH	CVen	zAUrnTCA
0.25	nan	26.7	60.13	90.4	70.0	18.9	39.8	15.92	14.54	26.11	nan
0.5	nan	20.4	125.4	21.4	42.1	nan	66.2	21.31	19.66	12.99	nan
1.0	nan	nan	189.9	25.8	16.98	nan	41.52	31.27	37.54	6.67	nan
2.0	nan	42.6	72.58	7.92	8.81	35.8	18.82	10.58	9.85	0.68	nan
4.0	nan	53.4	40.32	6.69	4.17	45.6	20.69	13.57	4.78	0.61	nan
8.0	nan	47.6	18.12	3.4	1.89	48.0	14.68	9.51	2.23	nan	nan
16.0	nan	43.2	31.3	6.7	0.945	35.3	5.06	1.82	1.48	nan	nan
24.0	1.912	35.9	0.65	3.26	nan	8.16	nan	nan	nan	nan	0.707
30.0	nan	25.0	nan	nan	nan	10.4	nan	nan	nan	nan	nan
48.0	3.555	nan	nan	nan	nan	1.229	nan	nan	nan	nan	1.176
72.0	3.76	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.292
96.0	3.803	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.304
120.0	3.84	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.307
144.0	3.855	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.308

TCE Oral Gavage 600.0 mg/kg

Hours	AUrnTCOGTCOH	CBldTCA	CFat	CKid	CLiv	CLivTCA	CLivTCOGTCOH	CLivTCOH	CTCOGTCOH	CTCOH	CVen	zAUrnTCA
0.25	nan	11.18	278.5	83.08	213.5	11.2	18.45	50.25	10.51	18.8	81.9	nan
0.5	nan	14.26	659.0	135.5	163.8	22.9	20.07	46.83	39.66	26.76	71.3	nan
2.0	nan	26.98	468.91	15.98	19.43	33.5	39.44	36.29	27.01	24.01	5.71	nan
4.0	nan	31.73	46.76	10.89	10.63	39.9	19.59	21.06	23.55	8.23	1.94	nan
8.0	nan	31.87	9.48	5.4	0.71	54.99	46.06	11.24	14.76	2.16	0.965	nan
12.0	nan	nan	nan	nan	nan	nan	nan	4.29	6.89	1.02	nan	nan
16.0	nan	29.48	0.71	nan	nan	39.06	nan	nan	nan	nan	nan	nan
24.0	6.892	24.81	0.32	0.42	0.339	28.2	nan	nan	nan	nan	nan	0.762
30.0	nan	nan	nan	nan	nan	15.2	nan	nan	nan	nan	nan	nan
40.0	nan	21.1	nan	nan	nan	7.6	nan	nan	nan	nan	nan	nan
48.0	9.072	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.683
72.0	9.593	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.867
96.0	9.716	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.904
120.0	9.829	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.927
144.0	9.895	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	1.941

TCE Oral Gavage 1200.0 mg/kg

Hours	AUrnTCOGTCOH	CBldTCA	CFat	CKid	CLiv	CLivTCA	CLivTCOGTCOH	CLivTCOH	CTCOGTCOH	CTCOH	CVen	zAUrnTCA
0.083	nan	nan	61.53	144.9	522.6	nan	nan	nan	nan	nan	165.87	nan
0.17	nan	nan	156.7	171.3	585.3	nan	nan	nan	nan	nan	191.31	nan
0.25	nan	16.5	567.2	265.6	499.4	11.09	23.67	65.35	62.12	18.83	123.52	nan
0.5	nan	23.1	826.0	282.6	408.0	16.95	23.3	75.33	63.13	27.73	86.9	nan
0.75	nan	29.2	865.3	1095.6	289.8	20.09	19.03	98.28	67.59	31.36	70.9	nan
1.0	nan	36.1	nan	690.1	228.8	26.02	34.89	105.3	50.86	35.42	43.08	nan
1.5	nan	41.8	1199.9	303.8	63.04	29.44	54.87	88.25	64.31	28.26	35.17	nan
2.0	nan	59.1	1050.5	109.8	38.97	35.65	62.31	92.24	95.02	41.86	20.36	nan
3.0	nan	64.0	550.2	32.4	nan	37.76	74.66	55.03	41.5	21.54	8.97	nan
4.0	nan	70.2	485.0	nan	26.5	42.07	76.92	57.64	46.7	24.64	7.5	nan
6.0	nan	94.1	219.2	40.2	15.37	43.92	26.66	35.96	51.86	4.589	nan	nan
8.0	nan	90.8	293.7	17.3	14.97	57.83	55.43	37.45	40.88	nan	1.64	nan
12.0	nan	nan	nan	nan	nan	nan	nan	nan	nan	4.487	0.72	nan
16.0	nan	65.2	4.4	3.6	12.86	27.71	nan	10.12	10.11	nan	0.47	nan
24.0	8.23	43.86	1.446	2.2	1.79	18.801	nan	nan	nan	nan	0.52	2.294
30.0	nan	41.48	nan	nan	nan	22.67	nan	nan	nan	nan	nan	nan
40.0	nan	9.15	nan	nan	nan	6.34	nan	nan	nan	nan	nan	nan

48.0	11.263	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.731
72.0	12.195	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	4.579
96.0	12.409	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	4.796
120.0	12.641	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	4.848
144.0	12.709	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	4.87

TCE Oral Gavage 2000.0 mg/kg

Hours	AUrnTCOGTCOH	CBldTCA	CFat	CKid	CLiv	CLivTCA	CLivTCOGTCOH	CLivTCOH	CTCOGTCOH	CTCOH	CVen	zAUrnTCA
0.25	nan	11.22	1152.0	636.0	1498.0	15.18	17.3	64.69	16.2	21.41	208.3	nan
0.5	nan	20.57	1993.0	652.0	335.0	27.58	14.47	73.45	22.88	32.94	162.0	nan
1.0	nan	30.34	4279.0	542.0	379.7	37.49	205.3	nan	41.84	140.1	nan	nan
2.0	nan	43.51	2015.0	176.0	116.2	49.46	237.98	nan	36.4	64.8	nan	nan
4.0	nan	63.43	1991.0	nan	114.5	65.32	66.23	114.88	61.1	29.14	48.6	nan
8.0	nan	nan	1503.0	139.4	105.1	105.65	23.04	73.96	40.88	nan	17.48	nan
16.0	nan	131.85	75.5	55.0	9.2	59.0	13.08	30.8	21.68	4.21	1.15	nan
24.0	15.28	51.38	7.4	1.3	2.0	44.6	nan	nan	nan	nan	nan	1.423
30.0	nan	54.57	nan	nan	nan	36.35	nan	nan	nan	nan	nan	nan
48.0	21.19	8.74	nan	nan	nan	9.98	nan	nan	nan	nan	nan	2.486
72.0	23.92	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.122
96.0	24.79	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.294
120.0	25.51	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.395
144.0	25.94	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.426
168.0	25.95	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.438
192.0	25.98	nan	nan	nan	nan	nan	nan	nan	nan	nan	nan	3.45

Abbas et al., 1997b

TCA IV 100.0 mg/kg

Hours	CBldTCA	zAUrnTCA
0.1	281.9	nan
0.15	380.3	nan
0.35	374.4	nan
0.65	207.0	nan
1.0	204.6	nan
2.0	94.3	nan
4.0	83.1	nan
8.0	48.97	nan
24.0	9.37	0.937
30.0	3.91	nan
48.0	nan	1.744
72.0	nan	1.801
96.0	nan	1.828
120.0	nan	1.843
144.0	nan	1.849
168.0	nan	1.853

TCOH IV 100.0 mg/kg

Hours	AUrnTCOGTCOH	CBldTCA	CTCOH
0.05	nan	0.83	77.34
0.1	nan	2.05	44.75
0.5	nan	2.21	19.11
1.0	nan	7.45	7.17
2.0	nan	21.1	0.163
24.0	1.093	nan	nan
48.0	1.859	nan	nan
72.0	1.986	nan	nan
96.0	2.097	nan	nan
120.0	2.061	nan	nan
144.0	2.071	nan	nan
168.0	2.1	nan	nan

TCE Inhalation 42.0 ppm for 4 hours -- females

Hours	CPlasTCA	CVen
2.0	17.69	0.306666667
3.83	23.94	0.34
4.167	29.92	nan
4.333	35.03	nan
4.5	24.33	nan
4.67	29.72	nan
6.0	25.18	nan
9.0	7.86	nan

TCE Inhalation 236.0 ppm for 4 hours -- females

Hours	CPlasTCA	CVen
2.0	50.8	4.58
3.83	57.2	4.95
4.5	nan	0.88
5.0	58.4	0.45
6.0	43.2	nan
7.0	24.0	nan
9.0	14.4	nan

TCE Inhalation 368.0 ppm for 4 hours -- females

Hours	CPlasTCA	CVen
2.0	58.5	5.9
3.83	59.8	6.3
4.33	61.7	1.03
4.67	69.9	0.8
5.0	59.7	0.22
5.33	57.7	nan
7.0	35.9	nan
10.0	24.5	nan
30.0	0.32	nan

Fisher et al., 1991

Data for CInhPPM were truncated in EPA (2011) file so they were digitized

TCE Inhalation 889.0 ppm for 4 hours -- females

Hours	CPlasTCA	CVen
2.0	51.1	3.9
3.83	83.2	3.6
4.167	90.9	2.0
4.333	92.3	1.4
4.5	94.1	0.72
5.0	94.3	0.55
6.0	76.7	nan
8.0	28.6	nan
26.0	0.46	nan

TCE Closed Chamber Inhalation 300.0 ppm for 4 hours -- females

Hours	CInhPPM
0.05	228.4977169
0.5	101.0376712
0.64	72.01027397
0.84	53.21689498
1.0	37.95890411
1.2	28.65525114
1.3	21.956621
1.5	17.11872146
1.7	12.28082192
1.8	9.48972
2.0	6.6

TCE Closed Chamber Inhalation 700.0 ppm for 4 hours -- females

Hours	CInhPPM
0.05	623.8
0.16	501.6
0.31	351.9
0.46	241.3
0.64	179.2
0.82	136.1
0.99	108.3
1.16	84.2
1.33	64.7
1.49	49.8
1.66	41.4
1.83	32.9
1.99	28.1
2.15	20.4
2.32	16.0
2.49	13.6
2.66	11.4

TCE Closed Chamber Inhalation 1100.0 ppm for 4 hours -- females

Hours	CInhPPM
0.05	949.6
0.16	782.4
0.30	563.1
0.48	443.2
0.63	377.5
0.82	304.7
0.99	265.5
1.15	231.9
1.30	191.1
1.47	157.5
1.66	137.5
1.81	119.9
1.98	102.3
2.16	84.3
2.32	69.5
2.50	59.3
2.65	51.7
2.82	42.7
2.99	35.2
3.18	29.0
3.32	22.8
3.49	19.5
3.64	16.0
3.81	13.2

TCE Closed Chamber Inhalation 3700.0 ppm for 4 hours -- females

Hours	CInhPPM
0.06	3424.2
0.14	2763.3
0.29	2174.9
0.48	1751.4
0.64	1529.7
0.79	1231.9
0.98	1204.0
1.13	1112.4
1.30	1051.6
1.47	937.8
1.64	916.6
1.81	916.6
1.98	895.8
2.16	846.9
2.32	800.6
2.49	782.4
2.64	764.7
2.98	706.5
3.14	690.5
3.29	674.9
3.48	659.6
3.63	659.6
3.82	588.3
3.97	574.9
4.16	574.9
4.31	543.5
4.49	513.8
4.66	502.2
4.81	474.7
5.00	447.8
5.16	423.3
5.33	400.2
5.50	369.8
5.68	348.8
6.00	287.4

TCE Closed Chamber Inhalation 7000.0 ppm for 4 hours -- females

Hours	CInhPPM
0.07	6263.1
0.14	5160.6
0.31	3928.6
0.48	3092.1
0.63	2700.7
0.80	2547.7
0.96	2353.9
1.13	2174.9
1.30	2056.0
1.47	2056.0
1.64	1939.5
1.79	1939.5
1.97	1939.5
2.14	1895.6
2.32	1833.5
2.49	1833.5
2.64	1792.0
2.79	1751.4

```
  2.98   1751.4
  3.14   1711.8
  3.32   1711.8
  3.47   1673.0
  3.64   1673.0
  3.81   1638.5
  3.96   1601.4
  4.15   1565.2
  4.30   1529.7
  4.47   1529.7
  4.97   1529.7
  5.16   1529.7
  5.31   1446.1
  5.49   1364.2
  5.66   1333.3
  5.81   1303.1
  5.98   1273.6
```

```
TCE Inhalation 110.0 ppm for 4 hours --
males
Hours, CPlasTCA, CVen
   2.0   17.76  1.5
   3.75  46.18  nan
   3.9   49.81  1.51
   4.2   38.99  0.38
   4.4    nan   0.38
   5.0   70.53  nan
   6.0   54.29  nan
   8.0   41.02  nan
  21.0    7.06  nan
```

```
TCE Inhalation 297.0 ppm for 4 hours --
males
Hours, CPlasTCA, CVen
   2.0    nan  1.48
   2.5   58.0  nan
   3.9    nan  1.2
   4.2  101.7  0.88
   4.4   88.5  0.37
   4.8  109.6  nan
   4.9  114.7  nan
   5.3   85.8  nan
   5.5   80.6  nan
   6.3   83.0  nan
  24.0    5.7  nan
```

```
TCE Inhalation 368.0 ppm for 4 hours --
males
Hours, CPlasTCA, CVen
   2.0    61.8  3.82
   3.9    94.2  3.72
   4.2   103.1  1.24
   4.4   103.0  0.51
   4.75   97.0  0.22
   5.0   101.4  nan
   5.5    71.6  nan
   6.5    58.8  nan
  24.0     9.8  nan];
```

```
TCE Inhalation 748.0 ppm for 4 hours --
males
Hours, CPlasTCA, CVen
   2.0    88.6  7.18
   3.9   127.4  7.2
   4.2   123.6  1.5
   4.4     nan  0.88
   4.5   123.6  0.49
   4.75  125.5  nan
   5.0   106.2  nan
   7.75   82.1  nan
   9.0    58.0  nan
  24.0     9.4  nan
```

```
TCE Closed Chamber Inhalation 1020.0 ppm for
   4 hours -- males
Hours, CInhPPM
  0.10   826.2
  0.19   613.6
  0.34   367.3
  0.52   219.4
  0.69   152.3
  0.84   100.8
  1.03   63.1
  1.18   41.3
  1.34   28.0
  1.50   17.9
  1.68   12.3
  1.85   8.6
  2.00   6.6
  2.17   5.1
  2.35   4.4
```

```
TCE Closed Chamber Inhalation 1800.0 ppm for
   4 hours -- males
Hours, CInhPPM
  0.18   1337.7
  0.26   1100.9
  0.35   906.0
  0.52   712.0
  0.69   599.6
  0.84   499.7
  1.02   388.6
  1.19   302.2
  1.36   243.1
  1.51   184.7
  1.69   128.3
  1.84   91.0
  2.02   62.4
  2.19   40.9
  2.34   27.1
  2.51   17.0
  2.68   11.5
  2.84   8.1
```

```
TCE Closed Chamber Inhalation 3800.0 ppm for
   4 hours -- males
Hours, CInhPPM
  0.18   2508.0
  0.35   1839.3
  0.52   1532.9
  0.69   1337.7
  0.85   1232.8
  1.00   1126.6
  1.19   1038.2
  1.36   970.9
  1.51   894.7
  1.69   826.2
  1.86   780.8
  2.03   737.8
  2.17   688.5
  2.34   635.9
  2.51   593.4
  2.68   541.1
  2.85   483.2
```

```
  3.02   440.7
  3.19   384.6
  3.35   342.7
  3.51   295.4
  3.69   257.8
  3.83   204.7
  4.02   161.2
  4.17   119.7
  4.33   88.0
  4.51   65.4
  4.68   49.0
  4.84   33.3
  5.03   22.3
  5.17   15.8
```

```
TCE Closed Chamber Inhalation 5600.0 ppm for
   4 hours -- males
Hours, CInhPPM
  0.10   5156.0
  0.19   4342.2
  0.35   3224.8
  0.52   2593.5
  0.69   2184.1
  0.84   1926.1
  1.02   1778.7
  1.17   1605.2
  1.35   1532.9
  1.51   1430.5
  1.69   1351.8
  1.86   1277.5
  2.01   1232.8
  2.17   1192.1
  2.34   1138.4
  2.51   1100.9
  2.67   1051.3
  2.76   1003.9
  2.93   981.1
  3.09   936.9
  3.26   885.4
  3.43   845.5
  3.59   826.2
  3.76   807.4
  3.94   789.0
  4.09   755.0
  4.26   712.0
  4.43   679.9
  4.60   650.7
  4.77   635.9
  4.94   607.2
  5.09   573.8
  5.27   548.0
```

```
TCE Closed Chamber Inhalation 10000.0 ppm
for
   4 hours -- males
Hours, CInhPPM
  0.09   8330.5
  0.18   7179.1
  0.35   5846.6
  0.52   5156.0
  0.69   4751.5
  0.85   4443.4
  1.03   4094.8
  1.19   3918.5
  1.35   3742.0
  1.52   3455.7
  1.70   3334.7
  1.85   3184.5
  2.03   3184.5
  2.18   3112.0
  2.36   3079.6
  2.52   2940.8
  2.69   2744.4
  2.85   2681.9
  3.02   2593.5
```

<u>Fisher and Allen, 1993</u>

```
TCE Oral Gavage 487.0 mg/kg -- females
Hours, CPlasTCA, CVen
   0.083   3.066666667  38.5
   0.17    5.466666667  24.33333333
   0.5    14.8          12.9
   1.0    25.4           6.233333333
   2.0    33.8           2.8
   4.0    55.63333333    nan
   7.0    56.56666667    nan
  24.0     2.2           nan
```

```
TCE Oral Gavage 973.0 mg/kg -- females
Hours, CPlasTCA, CVen
   0.083   5.39         22.1
   0.17    6.6          16.3
   0.25    7.0          35.8
   0.5    12.0          12.5
   1.0    20.16666667   17.88666667
   2.0    41.1          21.4
   3.0    41.2           nan
   4.0     nan          13.70666667
   7.0    43.7           nan
  27.0     5.466666667   nan
```

```
TCE Oral Gavage 1947.0 mg/kg -- females
Hours, CPlasTCA, CVen
   0.033   2.0   14.3
   0.083   5.1   38.6
   0.17   16.3   48.9
   0.25   15.2   42.5
   0.5    28.6   50.0
   1.0    33.0   27.9
   2.0    54.1  136.0
   3.0     nan  167.5
   4.0    89.3  119.8
   6.0    86.0   48.6
   8.0     nan    2.233333333
   9.0     nan   10.37333333
  24.0    14.6    nan
  30.0     4.0    nan
```

```
TCE Oral Gavage 487.0 mg/kg -- males
Hours, CPlasTCA, CVen
   0.083   5.8  50.9
   0.17    6.9  39.0
   0.5    17.9   nan
   1.0    32.0   6.9
   2.0    54.9   1.5
   7.0    82.2   nan
  24.0    13.8   nan
  30.0     4.1   nan
```

```
TCE Oral Gavage 973.0 mg/kg -- males
Hours, CPlasTCA, CVen
   0.033   8.933333333   9.7
   0.083  12.1          29.9
   0.17   11.8          50.9
   0.25   17.9          69.3
```

0.5	27.4	66.4
1.0	49.2	48.2
2.0	76.6	12.68666667
3.0	85.3	4.8
4.0	48.6	16.86666667
5.0	80.9	nan
6.0	86.4	nan
7.0	91.4	5.9
30.0	12.56666667	nan
48.0	2.0	nan

TCE Oral Gavage 1947.0 mg/kg -- males

Hours	CPlasTCA	CVen
0.033	1.2	20.0
0.083	3.9	30.7
0.17	11.9	45.1
0.25	16.3	64.7
0.5	32.7	71.7
1.0	61.6	127.3
2.0	41.3	33.26666667
3.0	56.1	106.7
4.0	54.9	75.7
5.0	61.1	103.4
6.0	91.0	47.9
7.0	94.4	23.9
24.0	47.5	nan
30.0	29.4	nan
48.0	28.5	nan
72.0	1.9	nan

Green and Prout, 1985

TCE Oral Gavage 10.0 mg/kg

Hours	AUrnTCOGTCOH	zAExhPost	zAUrnTCA
24.0	0.151246897	0.011115	0.023867144
72.0	nan	0.011115	nan

TCE Oral Gavage 500.0 mg/kg

Hours	AUrnTCOGTCOH	zAExhPost	zAUrnTCA
24.0	8.743811279	0.855	0.755310904
72.0	nan	0.855	nan

TCE Oral Gavage 1000.0 mg/kg

Hours	AUrnTCOGTCOH	zAExhPost	zAUrnTCA
24.0	11.99527586	4.9875	1.036993105
72.0	nan	4.9875	nan

TCE Oral Gavage 2000.0 mg/kg

Hours	AUrnTCOGTCOH	zAExhPost	zAUrnTCA
24.0	27.90858197	7.752	2.230208548
72.0	nan	7.752	nan

Greenberg et al., 1999

TCE Inhalation 100.0 ppm for 4 hours

Hours	CBldTCA	CFat	CKid	CLiv	CLivTCA	CLivTCOGTCOH	CLivTCOH	CTCOGTCOH	CTCOH	CVen
2.0	18.23	19.35	3.473	0.5719	12.84	18.52	4.134	4.51	2.041	0.6651
4.0	29.86	44.46	4.91	0.7577	21.17	22.91	4.446	6.222	1.847	0.8605
4.25	33.72	nan	nan	0.1673	21.81	13.73	1.162	2.733	1.778	0.1387
4.5	25.03	27.68	0.1341	0.051	16.32	5.328	5.099	1.97	0.7934	0.1497
4.75	31.63	nan	nan	nan	20.74	6.365	0.5918	2.09	0.3029	nan
6.0	27.06	nan	nan	nan	17.04	0.8768	0.4164	0.1985	0.0899	nan
12.0	6.798	nan	nan	nan	5.15	nan	nan	nan	nan	nan
18.0	3.992	nan	nan	nan	2.732	nan	nan	nan	nan	nan
28.0	1.908	nan	nan	nan	1.404	nan	nan	nan	nan	nan

TCE Inhalation 600.0 ppm for 4 hours

Hours	CBldTCA	CFat	CKid	CLiv	CLivTCA	CLivTCOGTCOH	CLivTCOH	CTCOGTCOH	CTCOH	CVen
2.0	56.1	244.48	22.85	10.19	33.72	36.6	28.93	16.17	16.53	6.851
4.0	96.66	233.7	22.04	12.62	52.12	62.08	24.7	25.1	13.37	7.325
4.25	74.62	198.4	6.167	3.013	45.67	49.31	17.65	17.87	10.89	1.534
4.5	99.03	167.5	4.714	1.074	54.97	19.37	5.476	6.746	3.979	0.5987
4.75	77.74	142.2	2.855	0.6447	48.54	30.51	6.282	8.252	3.201	0.4649
6.0	107.67	104.1	0.6404	0.2754	48.74	4.313	2.647	2.028	1.007	0.1699
12.0	25.82	nan	nan	nan	13.01	nan	nan	0.3544	nan	nan
18.0	13.34	nan	nan	nan	7.952	nan	nan	nan	nan	nan
28.0	7.191	nan	nan	nan	4.405	0.1568	nan	nan	nan	nan
47.0	0.8069	nan	nan	nan	0.7298	0.1025	nan	nan	nan	nan

Larson and Bull, 1992a

TCE Oral Gavage 197.25 mg/kg

Hours	CBldMix	CBldTCA	CTCOH
0.25	44.8074	22.876	28.24055
0.75	20.8926	35.131	19.4051
2.0	nan	24.3466	nan
8.0	nan	20.5884	nan
24.0	nan	2.451	nan

TCE Oral Gavage 591.75 mg/kg

Hours	CBldMix	CBldTCA	CTCOH
0.25	151.11	14.0524	25.415
0.75	74.03076	36.4382	32.89
2.0	30.11688	63.0724	37.375
8.0	nan	100.8178	nan
24.0	nan	6.6994	nan

TCE Oral Gavage 1972.5 mg/kg

Hours	CBldMix	CBldTCA	CTCOH
0.25	436.3794	22.876	38.3617
0.75	292.8906	42.9742	34.8634
2.0	154.9206	68.4646	59.8897
8.0	4.0734	122.3866	17.98485
24.0	nan	28.2682	nan
48.0	nan	4.7386	nan

Larson and Bull, 1992b

TCA Oral Gavage 20.0 mg/kg

Hours	CPlasTCA
0.25	35.131
1.0	33.6604
3.0	33.6604
5.0	23.5296
10.0	9.1504
16.0	4.085

TCA Oral Gavage 100.0 mg/kg

Hours	CPlasTCA
0.25	104.576
1.0	119.9356
3.0	109.8048
5.0	89.7066
10.0	49.02
16.0	7.6798
24.0	5.2288

Merdink et al., 1998

TCE IV 100.0 mg/kg

Hours	CBldTCA	TotCTCOH
0.18	6.0458	7.13115
0.359	9.5589	5.8006
0.525	9.86936	3.6179
0.65	12.69618	2.40695
0.76	13.10468	2.6013
1.02	16.34	2.3322
1.26	18.791	0.79534
1.52	16.07856	0.617435
2.99	18.3008	0.192855
6.01	15.09816	nan

Prout et al., 1985

Data were truncated in EPA (2011) file so they were digitized

TCE Oral Gavage 1000 mg/kg

Hours	CBldMix	CBldTCA	TotCTCOH	zAExhPost
0.25	10.3	nan	nan	nan
0.3	nan	nan	9.6	nan
0.5	18.0	nan	21.7	0.74
0.75	13.6	39.0	29.4	nan
1.0	8.0	106.0	27.8	1.34
1.5	10.5	nan	30.6	1.78
2.0	6.2	69.0	27.6	2.18
2.5	nan	146.0	20.3	2.59
3.0	6.3	121.0	nan	nan
3.5	1.5	nan	9.5	2.88
4.0	1.7	157.0	10.7	3.04
4.5	1.8	133.0	14.3	3.09
5.0	2.2	149.0	2.8	3.1
5.5	2.3	101.0	7.4	3.15
6.0	2.9	121.0	6.6	3.17
6.5	3.3	nan	5.5	3.19
7.0	4.3	162.0	2.6	3.17
7.5	1.9	196.0	1.5	3.24
8.0	nan	211.0	0.7	3.24
8.5	nan	nan	nan	3.25
9.0	nan	201.0	nan	3.27
10.0	nan	190.0	nan	nan
11.0	nan	189.0	nan	nan
12.0	nan	170.0	nan	nan
13.0	nan	260.0	nan	nan
14.0	nan	242.0	nan	nan
15.0	nan	216.0	nan	nan
16.0	nan	179.0	nan	nan
17.0	nan	118.0	nan	nan
18.0	nan	59.0	nan	nan
19.0	nan	124.0	nan	nan
20.0	nan	197.0	nan	nan
21.0	nan	169.32	nan	nan
22.0	nan	144.87	nan	nan
24.0	nan	237.29	nan	nan
25.0	nan	223.79	nan	nan
27.0	nan	156.10	nan	nan
28.0	nan	149.35	nan	nan
29.0	nan	266.63	nan	nan
30.0	nan	284.67	nan	nan
32.0	nan	68.91	nan	nan
33.0	nan	55.41	nan	nan
34.0	nan	28.35	nan	nan
36.0	nan	39.64	nan	nan
38.0	nan	28.35	nan	nan
41.0	nan	18.57	nan	nan
44.0	nan	5.76	nan	nan

Templin et al., 1993

TCE Oral Gavage 500 mg/kg

Hours	CBldMix	CBldTCA	CTCOH
0.25	28.3824	10.7844	17.9101
0.5	24.7032	18.791	27.7771
0.75	21.9438	25.0002	35.5511
1.0	11.826	41.667	40.2454
1.5	3.8106	46.569	30.199
2.0	1.7082	43.4644	8.56635
3.0	nan	57.19	0.73255
4.0	nan	64.8698	nan
6.0	nan	39.7062	nan
9.0	nan	37.2552	nan
12.0	nan	30.8826	nan
18.0	nan	10.7844	nan
24.0	nan	8.8236	nan
36.0	nan	1.9608	nan

APPENDIX I. DATA FOR RAT VALIDATION FIGURES

The following data are for generating rat validation figures in Appendix B.

Bernauer et al., 1996

```
TCE Inhalation 40.0 ppm for 6 hours
Hours, AUrnTCOGTCOH, zAUrnNDCVC, zAUrnTCA
  12.0  0.85181  0.0004626  0.055668
  24.0  0.97350  0.0010022  0.055668
  36.0  1.09519  0.0015612  0.055668
  48.0  1.15603  0.0021395  0.055668
```

```
TCE Inhalation 80.0 ppm for 6 hours
Hours, AUrnTCOGTCOH, zAUrnNDCVC, zAUrnTCA
  12.0  1.70363  0.0005107  0.11134
  24.0  2.06869  0.0009926  0.16700
  36.0  2.31207  0.0014937  0.16700
  48.0  2.43375  0.0020333  0.16700
```

```
TCE Inhalation 160.0 ppm for 6 hours
Hours, AUrnTCOGTCOH, zAUrnNDCVC, zAUrnTCA
  12.0  2.79882  0.0006360  0.33401
  24.0  3.16388  0.0016190  0.55668
  36.0  3.46810  0.0027754  0.66802
  48.0  3.71147  0.0036041  0.72368
```

Dallas et al., 1991

Data were truncated in EPA (2011) file so they were digitized

```
TCE Inhalation 50.0 ppm for 2 hours
Hours, CArt, CMixExh
  0.035   0.205   0.126
  0.065   0.264   0.146
  0.105   0.336   0.161
  0.14    0.442   nan
  0.175   0.401   0.155
  0.26    0.452   0.178
  0.335   0.488   0.175
  0.42    0.352   nan
  0.505   0.491   0.174
  0.68    nan     0.18
  0.76    0.437   nan
  0.85    nan     0.172
  1.01    0.556   0.179
  1.18    nan     0.187
  1.25    0.517   nan
  1.35    nan     0.183
  1.51    0.643   0.193
  1.68    nan     0.184
  1.76    0.597   nan
  1.84    nan     0.18
  2.005   0.607   0.176
  2.02    nan     0.062
  2.04    0.341   0.033
  2.075   0.272   0.03
  2.11    0.264   0.007
  2.14    0.161   nan
  2.17    0.225   0.014
  2.25    0.15    0.012
  2.33    0.161   nan
  2.42    0.099   nan
  2.5     0.127   0.008
  2.75    0.086   0.005
  3.0     0.076   0.005
  3.255   0.055   0.003
  3.5     0.045   0.001
  3.755   0.037   nan
  4.005   0.027   0.001
  4.5     0.014   nan
```

```
TCE Inhalation 500.0 ppm for 2 hours
Hours, CArt, CMixExh
  0.02    nan     1.258
  0.04     3.08   nan
  0.06     4.51   1.445
  0.095    4.77   1.492
  0.13     7.04   nan
  0.17     7.29   1.57
  0.25     7.7    1.616
  0.335   10.12   1.6
  0.42    11.19   nan
  0.5     12.12   1.73
  0.67     nan    1.725
  0.75    13.56   nan
  0.84     nan    1.788
  1.01    15.3    1.824
  1.18     nan    1.839
  1.25    14.54   nan
  1.34     nan    1.73
  1.505   15.41   1.839
  1.67     nan    1.819
  1.76    15.3    nan
  1.84     nan    1.912
  2.015   17.16   0.697
  2.04    12.79   nan
  2.065   12.48   0.531
  2.09     nan    0.468
  2.11    11.45   0.4
  2.14    10.42   nan
  2.175   10.12   0.385
  2.255    8.88   0.359
  2.34     7.5    nan
  2.43     7.39   nan
  2.51     6.67   0.224
  2.755    5.64   0.161
  3.01     3.39   0.104
  3.26     2.62   0.083
  3.51     1.84   0.068
  3.75     1.59   0.032
  4.005    1.33   0.037
  4.505    0.86   0.043
  5.0      0.76   0.026
```

Fisher et al., 1989

Data were truncated in EPA (2011) file so they were digitized

```
TCE Closed Chamber Inhalation 300.0 ppm
Hours, CInhPPM
  0.083  214.0
  0.5     99.0
  0.667   70.3
```

```
  0.833   52.3
  1.0     38.1
  1.167   14.0
  1.333   11.0
  1.5      8.0
```

```
TCE Closed Chamber Inhalation 1100.0 ppm
Hours, CInhPPM
  0.04   1067.1
  0.09    939.0
  0.19    752.3
  0.35    550.0
  0.53    420.4
  0.69    322.1
  0.87    264.2
  1.03    216.7
  1.20    177.7
  1.37    154.7
  1.53    133.0
  1.70    115.6
  1.87    100.6
  2.02     82.5
  2.20     69.3
  2.35     57.6
  2.52     46.7
  2.69     37.0
```

```
TCE Closed Chamber Inhalation 2200.0 ppm
Hours, CInhPPM
  0.05   2169.8
  0.11   1929.8
  0.19   1620.3
  0.35   1331.8
  0.53   1092.4
  0.69    927.0
  0.87    796.9
  1.04    685.0
  1.20    596.4
  1.37    537.2
  1.53    489.1
  1.70    436.0
  1.86    410.7
  2.03    383.6
  2.19    361.4
  2.36    337.6
  2.52    310.7
  2.69    290.2
  2.86    270.5
  3.03    255.3
  3.20    238.0
  3.36    227.1
  3.53    211.7
  3.69    195.2
  3.85    180.0
  4.01    171.8
  4.18    162.2
  4.35    151.2
  4.52    139.4
  4.67    125.6
  4.86    113.1
  5.01    101.7
```

```
TCE Closed Chamber Inhalation 5100.0 ppm
Hours, CInhPPM
  0.04   5013.9
  0.11   4459.3
  0.19   3882.4
  0.36   3077.6
  0.53   2551.3
  0.70   2119.5
  0.87   1760.8
  1.02   1529.7
  1.19   1331.8
  1.36   1212.6
  1.53   1067.1
  1.70    984.1
  1.86    917.2
  2.02    845.9
  2.18    796.9
  2.36    762.0
  2.52    734.9
  2.69    693.8
  2.86    670.5
  3.03    646.7
  3.20    631.7
  3.35    625.0
  3.52    596.4
  3.68    582.5
  3.85    576.4
  4.01    563.0
  4.18    555.9
  4.35    537.2
  4.51    530.4
  4.68    519.2
  4.86    507.2
  5.01    500.7
  5.18    489.1
  5.35    489.1
  5.52    455.9
  5.68    455.9
  5.86    440.6
  6.02    436.0
```

Fisher et al., 1991

```
TCE Inhalation 600.0 ppm for 4 hours --
females
Hours, CBldTCA, CPlasTCA, CVen
   0.6    1.672   2.2   9.3
   3.75  15.656  20.6  26.4
   4.25  14.972  19.7  19.7
   5.0   24.016  31.6   6.9
   6.0   25.232  33.2   3.5
   8.75  29.564  38.9   nan
  26.0    8.284  10.9   nan
  32.0    4.484   5.9   nan
  48.0    0.988   1.3   nan
```

```
TCE Inhalation 505.0 ppm for 4 hours --
males
Hours, CBldTCA, CPlasTCA
   2.0    4.94    6.5
   3.75   8.284  10.9
   6.0   16.948  22.3
   8.0   16.34   21.5
  10.0   15.352  20.2
  12.0   13.3    17.5
  26.0    4.788   6.3
  32.0    3.42    4.5
```

Green and Prout, 1985

```
TCA IV 10.0 mg/kg
Hours, AUrnTCTot_Mole
  24.0  0.004011628
```

```
TCA Oral Gavage 75.0 mg/kg
Hours, AUrnTCTot_Mole
  24.0  0.05119186


TCE Oral Gavage 500.0 mg/kg
Hours, AUrnTCOGTCOH, zAUrnTCA
  24.0  44.79732  3.42357


TCA IV 10.0 mg/kg with bile cannulation
Hours, AUrnTCTot_Mole, zABileTCOG
  24.0  0.18798  18.35018
```

Hissink et al., 2002

```
Data were truncated in EPA (2011) file so
they were digitized


TCE IV 10.0 mg/kg
Hours, AUrnTCTot_Mole, CVen
    0.25   nan     3.439
    0.5    nan      1.938
    1.0    nan      0.574
    1.5    nan      0.274
    2.0    nan      0.161
    3.0    nan      0.060
    4.0    nan      0.021
    6.0    0.0101   0.009
    8.0    nan      0.003
   12.0    0.0119   nan
   24.0    0.0128   nan
   48.0    0.0131   nan
   72.0    0.0133   nan
   96.0    0.0133   nan
  120.0    0.0133   nan
  144.0    0.0133   nan
  168.0    0.0133   nan


TCE IV 75.0 mg/kg
Hours, AUrnTCTot_Mole, CVen
    0.25  nan      46.89
    0.5   nan      31.28
    1.0   nan      14.10
    1.5   nan       6.54
    2.0   nan       3.73
    3.0   nan       1.55
    4.0   nan       0.67
    6.0   0.0568    0.27
    8.0   nan       0.09
   12.0   0.0751    nan
   24.0   0.0835    nan
   48.0   0.0856    nan
   72.0   0.0860    nan
   96.0   0.0864    nan
  120.0   0.0866    nan
  144.0   0.0868    nan
  168.0   0.0871    nan


TCE Oral Gavage 100.0 mg/kg
Hours, AUrnTCTot_Mole, CVen
    0.25   nan     5.56
    0.5    nan     6.42
    1.0    nan     5.27
    1.5    nan     4.44
    2.0    nan     3.48
    3.0    nan     1.66
    4.0    nan     0.65
    6.0    0.081   0.14
    8.0    nan     0.08
   12.0    0.144   nan
   24.0    0.165   nan
   48.0    0.170   nan
   72.0    0.171   nan
   96.0    0.171   nan
  120.0    0.172   nan
  144.0    0.172   nan
  168.0    0.173   nan


TCE Oral Gavage 1000.0 mg/kg
Hours, AUrnTCTot_Mole, CVen
    0.25   nan     67.11
    0.5    nan     52.67
    1.0    nan     43.22
    1.5    nan     41.68
    2.0    nan     37.08
    3.0    nan     43.65
    4.0    nan     53.20
    6.0    0.062   63.67
    8.0    nan     53.20
   12.0    0.263    nan
   24.0    0.654    0.17
   48.0    0.763    nan
   72.0    0.774    nan
   96.0    0.780    nan
  120.0    0.785    nan
  144.0    0.785    nan
  168.0    0.794    nan
```

Kaneko et al., 1994

```
TCE Inhalation 50.0 ppm for 6 hours
Hours, AUrnTCOGTCOH, CVen, zAUrnTCA
   6.0  0.37375  0.3850   0.008938
   8.0  nan      0.09027  nan
  10.0  nan      0.02549  nan
  12.0  0.74302  nan      0.033987
  24.0  0.84916  nan      0.061929
  48.0  0.89102  nan      0.137910


TCE Inhalation 100.0 ppm for 6 hours
Hours, AUrnTCOGTCOH, CVen, zAUrnTCA
   6.0  0.78189  0.77263  0.015507
   8.0  nan      0.24835  nan
  10.0  nan      0.05453  nan
  12.0  1.36643  nan      0.086112
  24.0  1.48902  nan      0.189544
  48.0  1.50995  nan      0.29412


TCE Inhalation 500.0 ppm for 6 hours
Hours, AUrnTCOGTCOH, CVen, zAUrnTCA
   6.0  1.5249   5.11146  0.06291
   8.0  nan      1.21545  nan
  10.0  nan      0.33770  nan
  12.0  3.72255  nan      0.32843
  24.0  4.23085  nan      0.61765
  48.0  4.3654   nan      0.86112


TCE Inhalation 1000.0 ppm for 6 hours
Hours, AUrnTCOGTCOH, CVen, zAUrnTCA
   6.0  1.8239   29.565   0.08562
   8.0  nan      11.60262  nan
  10.0  nan       4.6647   nan
  12.0  4.23085   1.78704  0.4902
  24.0  5.5913    nan      1.19772
```

48.0	5.96505	nan	1.62583

Keys et al., 2003

Data were truncated in EPA (2011) file so they were digitized

TCE Intra-arterial 8.0 mg/kg

Hours	CFat	CGut	CKid	CLiv	CMus	CVen
0.1	12.36	3.13	2.98	5.63	2.33	3.41
0.2	nan	2.78	2.22	3.72	2.11	2.39
0.3	nan	1.57	0.61	nan	1.20	0.88
0.4	30.88	nan	nan	1.19	nan	nan
0.5	22.18	0.18	0.29	0.43	0.27	0.55
0.7	nan	0.49	0.21	nan	nan	nan
0.8	nan	nan	nan	0.30	0.42	0.18
1.0	18.09	0.34	0.08	0.13	0.22	0.08
1.5	12.36	0.17	0.07	0.13	0.13	0.07
2.0	14.03	0.09	0.04	0.05	0.13	0.04
2.5	8.00	0.05	0.02	0.03	0.06	0.02
4.0	4.56	nan	nan	nan	nan	nan
6.0	3.46	nan	nan	nan	nan	nan
8.0	2.19	nan	nan	nan	nan	nan
12.0	0.71	nan	nan	nan	nan	nan
16.0	0.19	nan	nan	nan	nan	nan
18.0	0.01	nan	nan	nan	nan	nan
24.0	0.01	nan	nan	nan	nan	nan

TCE Inhalation 50.0 ppm for 2 hours

Hours	CFat	CGut	CKid	CLiv	CCMus	CVen
0.1	1.75	0.668	1.338	0.643	0.523	1.637
0.2	nan	nan	nan	nan	nan	nan
0.3	5.49	nan	1.214	nan	nan	0.967
0.4	nan	0.885	nan	0.466	0.653	nan
0.7	10.13	1.016	1.497	0.527	0.912	0.844
1.0	16.14	1.320	1.646	0.740	1.277	1.053
1.5	11.88	0.899	1.214	0.423	0.740	0.905
2.0	10.85	0.899	0.884	0.382	0.530	1.034
2.1	13.45	nan	0.405	0.102	0.436	0.435
2.2	nan	0.591	0.373	0.168	0.295	0.406
2.3	11.61	0.338	0.228	0.100	nan	0.332
2.5	11.47	0.310	0.153	0.079	0.236	0.213
2.8	10.13	0.294	0.166	0.074	0.227	0.104
3.0	8.17	0.157	0.113	0.067	0.131	0.103
3.5	9.80	0.107	0.050	0.041	0.113	0.026
4.0	3.33	0.134	0.053	0.043	0.116	0.049
5.0	5.49	nan	nan	nan	nan	0.017

TCE Inhalation 50.0 ppm for 2 hours

Hours	CFat	CGut	CKid	CLiv	CCMus	CVen
0.083	19.11	nan	14.41	18.21	5.96	6.25
0.333	66.29	nan	18.92	23.89	10.08	10.28
1.0	186.12	nan	20.26	27.61	15.03	11.50
2.0	323.98	nan	24.91	31.54	17.40	17.68
2.083	266.28	14.987	11.50	13.56	9.14	11.81
2.25	493.96	16.831	11.18	13.18	8.87	8.57
2.75	269.57	7.856	5.18	4.34	4.55	3.12
3.5	298.91	3.803	3.47	2.08	1.59	2.21
5.0	150.91	0.876	0.85	0.25	1.11	0.61

TCE Oral Gavage 8.0 mg/kg

Hours	CFat	CGut	CKid	CLiv	CCMus	CVen
0.1	15.49	3.35	3.55	5.93	2.80	3.76
0.2	34.93	2.94	2.65	3.63	2.37	2.59
0.3	nan	1.70	0.99	1.41	1.33	1.04
0.5	33.49	0.25	0.38	0.53	0.35	0.52
0.75	nan	0.61	0.30	0.38	0.57	0.23
1.0	19.26	0.39	0.13	0.19	0.31	0.12
1.5	24.46	0.21	0.09	0.14	0.16	0.09
2.0	14.59	0.11	0.04	0.05	0.06	0.03
3.0	8.91	0.06	0.03	0.04	0.07	0.02
4.0	5.13	nan	nan	nan	nan	nan
6.0	3.73	nan	nan	nan	nan	nan
8.0	2.36	nan	nan	nan	nan	nan
12.0	0.81	nan	nan	nan	nan	nan
18.0	0.03	nan	nan	nan	nan	nan
24.0	0.03	nan	nan	nan	nan	nan

Kimmerle73_Rat.m

```
TCE Inhalation 49.0 ppm for 4 hours
Hours, AUrnTCOGTCOH, zAExhPost, zAUrnTCA
   5.0  nan     0.0511  nan
   6.0  nan     0.0635  nan
   7.0  nan     0.0738  nan
   8.0  nan     0.0827  nan
  28.0  0.848   nan     0.3425
  52.0  0.8591  nan     0.4252


TCE Inhalation 54.0 ppm for 4 hours
Hours, CTCOH
  4.0833  0.8
  4.5     0.3
  5.0     0.2


TCE Inhalation 175.0 ppm for 4 hours
Hours, AUrnTCOGTCOH, zAExhPost, zAUrnTCA
   5.0  nan     0.3941  nan
   6.0  nan     0.5094  nan
   7.0  nan     0.5551  nan
   8.0  nan     0.5777  nan
   9.0  nan     0.5923  nan
  10.0  nan     0.5995  nan
  11.0  nan     0.6055  nan
  12.0  nan     0.6113  nan
  28.0  2.2852  nan     0.8618
  52.0  2.306   nan     1.0076
  76.0  2.3092  nan     1.0373


TCE Inhalation 330.0 ppm for 4 hours
Hours, AUrnTCOGTCOH, zAExhPost, zAUrnTCA
   5.0  nan     3.87   nan
   6.0  nan     4.445  nan
   7.0  nan     4.624  nan
   8.0  nan     4.711  nan
   9.0  nan     4.757  nan
  10.0  nan     4.783  nan
  11.0  nan     4.807  nan
  12.0  nan     4.824  nan
  28.0  4.0664  nan    1.0291
  52.0  4.0828  nan    1.2373
  76.0  4.0851  nan    1.2713


TCE Inhalation 3160.0 ppm for 4 hours
Hours, CTCOH, CVen
  4.0833  1.74  89.2
  4.5     1.68  35.4
  5.0     1.75  19.4
```

Larson and Bull, 1992a

```
TCA Oral Gavage 20.0 mg/kg
Hours, CPlasTCA
   0.25  17.3204
   1.0   36.765
   3.0   36.1114
   5.0   30.229
  10.0   16.8302
  16.0    8.0066
  24.0    4.4118


TCA Oral Gavage 100.0 mg/kg
Hours, CPlasTCA
   0.25   85.1314
   1.0   202.2892
   3.0   147.5502
   5.0   107.6806
  10.0    57.3534
  16.0    26.144
  24.0    10.621
  32.0     4.4118
```

Larson and Bull, 1992b

```
TCE Oral Gavage 197.25 mg/kg
Hours, CBldTCA, CTCOH, CVen
   1.0   6.0458  1.196    11.18214
   2.0   8.17    2.37705   6.42546
   4.0  12.7452  2.392     2.50974
   8.0  13.2354  0.61295   1.14318
  12.0  10.621   0.1495    nan
  24.0   2.1242  nan       nan];


TCE Oral Gavage 591.75 mg/kg
Hours, CBldTCA, CTCOH, CVen
   1.0   2.7778   1.30065  25.8201
   2.0   6.76476  1.59965  34.40052
   4.0   9.08504  2.43685  20.1699
   8.0  20.16356  4.44015   6.74082
  12.0  24.49366  1.92855   3.23244
  24.0  17.18968  0.43355   nan
  48.0   1.53596  nan       nan


TCE Oral Gavage 3024.0 mg/kg
Hours, CBldTCA, CTCOH, CVen
   1.0   4.2484  1.794    61.6266
   2.0   9.804   2.99    164.5128
   4.0  11.1112  2.99    101.178
   8.0  23.5296  3.289    88.1694
  12.0  36.6016  5.083    46.2528
  24.0  60.6214  3.4385    6.4386
  48.0   5.5556  nan       nan
```

Lee et al., 2000

```
TCE IV 16.0 mg/kg
Hours, CBldMix, CLiv
  0.01111  16.0  20.0
  0.01944  25.0  22.0
  0.03611  20.0  41.0
  0.08611  11.0  17.0


TCE Portal vein IV 16.0 mg/kg
Hours, CBldMix, CLiv
  0.01111  19.0   82.0
  0.01944  25.0  209.0
  0.03611  15.0   44.0
  0.08611   8.0   14.0
```

Merdink et al., 1999

```
TCOH IV 100.0 mg/kg
Hours, CTCOH
  3.274  182.39
  3.509  130.5135
  4.01    72.059
  4.99    41.86
  6.0     28.2555
  8.01    14.4417
```

Prout et al., 1985

Data were truncated in EPA (2011) file so they were digitized

Data for exhaled air in the paper were individual data but EPA (2011) plots single values so the values from EPA (2011) were digitized

TCE Oral Gavage 1000.0 mg/kg – rats not specified

Hours	CArt	CBldTCA	CTCOH	zAExhPost
0.25	5.95	nan	nan	nan
0.5	20.37	nan	nan	3.32207
0.75	25.47	nan	nan	nan
1.0	nan	nan	0.80	5.70037
1.5	20.51	nan	0.99	8.85364
2.0	24.32	nan	0.95	11.3451
2.5	42.32	2.38	0.75	15.36911
3.0	61.84	nan	0.85	19.92356
3.5	nan	nan	0.85	26.12868
4.0	43.35	nan	1.09	33.48141
4.5	40.92	3.14	1.15	39.65263
5.0	29.18	9.13	0.80	43.80743
5.5	29.04	nan	1.09	48.50986
6.0	28.79	9.89	0.80	53.71706
6.5	nan	nan	1.24	56.78925
7.0	20.77	14.43	0.61	58.79797
7.5	nan	nan	1.39	64.35948
8.0	18.60	15.19	0.51	68.83329
8.5	nan	nan	nan	71.93171
9.0	12.73	25.73	1.59	nan
10.0	10.93	17.46	7.28	79.65309
10.5	nan	nan	nan	85.19
11.0	7.49	nan	1.97	85.19
11.5	nan	nan	nan	89.23123
12.0	nan	44.53	2.17	nan
13.0	nan	36.20	1.24	nan
14.0	nan	48.66	0.61	nan
15.0	nan	nan	2.07	nan
16.0	nan	26.83	0.75	nan
17.0	nan	nan	0.85	nan
18.0	nan	34.34	0.65	nan
19.0	nan	43.77	nan	nan
20.0	nan	39.64	nan	nan
22.0	nan	23.46	nan	nan
23.0	nan	18.15	nan	nan
25.0	nan	13.68	nan	nan
26.0	nan	13.26	nan	nan
28.0	nan	21.60	nan	nan
29.0	nan	32.06	nan	nan
30.0	nan	38.13	nan	nan
32.0	nan	31.72	nan	nan
33.0	nan	17.81	nan	nan
35.0	nan	19.67	nan	nan
36.0	nan	23.80	nan	nan
37.0	nan	21.60	nan	nan
40.0	nan	5.76	nan	nan

TCE Oral Gavage 10.0 mg/kg – Alderley Park Wistar

Hours	AUrnTCTot_Mole	zAExhPost
24.0	0.007894977	0.019
48.0	0.008314307	0.019
72.0	0.008429985	nan

TCE Oral Gavage 500.0 mg/kg – Alderley Park Wistar

Hours	AUrnTCTot_Mole	zAExhPost
24.0	0.180022831	47.405
48.0	0.18869863	47.405
72.0	0.191590563	nan

TCE Oral Gavage 1000.0 mg/kg – Alderley Park Wistar

Hours	AUrnTCTot_Mole	zAExhPost
24.0	0.247260274	98.99
48.0	0.264611872	98.99
72.0	0.270395738	nan

TCE Oral Gavage 10.0 mg/kg – Osborne-Mendel

Hours	AUrnTCTot_Mole	zAExhPost
24.0	0.009586758	0.0247
72.0	0.010035008	0.0247

TCE Oral Gavage 500.0 mg/kg – Osborne-Mendel

Hours	AUrnTCTot_Mole	zAExhPost
24.0	0.297869102	40.565
72.0	0.3152207	40.565

TCE Oral Gavage 1000.0 mg/kg – Osborne-Mendel

Hours	AUrnTCTot_Mole	zAExhPost
24.0	0.422222222	106.78
72.0	0.449695586	106.78

TCE Oral Gavage 2000.0 mg/kg – Osborne-Mendel

Hours	AUrnTCTot_Mole	zAExhPost
24.0	0.38173516	295.64
72.0	0.404870624	295.64

Simmons et al., 2002

Data for CInhPPM were truncated in EPA (2011) file so they were digitized

TCE Inhalation 200.0 ppm for 5 hours

Hours	CFat	CLiv	CVen
0.083	1.6	0.875	0.79
0.333	4.875	1.275	1.29
1.0	23.0	1.5	1.2
2.0	11.1	0.015	0.14

TCE Inhalation 2000.0 ppm for 5 hours

Hours	CFat	CLiv	CVen
0.083	13.5	24.0	9.35
0.333	8.45	42.0	12.15
1.0	256.667	79.0	40.75
2.0	245.0	8.4	4.75

TCE Inhalation 4000.0 ppm for 5 hours

Hours	CFat	CLiv	CVen
0.083	20.4	69.0	31.5
0.333	200.0	140.0	70.75
1.0	595.875	189.025	57.05
2.0	670.0	55.0	31.75

TCE Closed Chamber Inhalation 108.0 ppm

Hours	CInhPPM
0.02	106.64
0.18	95.78
0.34	84.01

0.49	77.40
0.67	69.52
0.83	63.93
1.00	59.55
1.18	54.76
1.34	50.92
1.51	47.43
1.68	44.18
1.83	41.60
1.99	38.26
1.99	38.26
2.17	36.09
2.33	33.56
2.49	31.66
2.66	29.43
2.84	27.77
3.01	24.94
3.17	23.79
3.34	22.93
3.50	21.60
3.67	20.34
3.84	18.74
4.00	17.84
4.17	17.01
4.32	16.02

TCE Closed Chamber Inhalation 506.0 ppm

Hours,	CInhPPM
0.02	502.19
0.19	456.83
0.35	400.70
0.51	364.50
0.68	347.01
0.83	315.66
1.02	280.43
1.19	264.07
1.34	242.86
1.50	226.21
1.69	213.02
1.84	191.32
2.01	175.95
2.18	165.99
2.35	156.31
2.51	141.93
2.68	137.10
2.85	126.09
3.01	117.44
3.17	110.59
3.34	101.71
3.51	97.01
3.69	92.52
3.85	84.01
4.00	79.25
4.18	74.63
4.33	68.64
4.51	64.63
4.69	58.79
4.84	52.80
5.01	49.19
5.17	46.91
5.34	43.62
5.51	41.15
5.69	38.75
5.85	36.49

TCE Closed Chamber Inhalation 864.0 ppm

Hours,	CInhPPM
0.02	859.32
0.20	771.78
0.35	685.64
0.52	630.55
0.70	587.33
0.84	546.07
1.01	515.16
1.18	490.45
1.35	456.83
1.51	435.70
1.69	415.56
1.83	395.62
2.01	373.23
2.17	359.88
2.33	338.89
2.51	319.71
2.68	308.28
2.85	297.25
3.01	276.88
3.17	273.87
3.33	257.90
3.51	254.63
3.68	237.18
3.84	228.69
4.01	220.92
4.20	210.70
4.34	200.59
4.51	184.81
4.69	180.16
4.84	174.03
5.01	165.99
5.19	154.33
5.35	147.19
5.52	138.61
5.70	130.76
5.85	123.14

TCE Closed Chamber Inhalation 2940.0 ppm

Hours,	CInhPPM
0.02	2899.98
0.20	2765.89
0.35	2511.44
0.52	2284.56
0.70	2127.95
0.85	1978.48
1.02	1886.99
1.18	1757.64
1.35	1676.37
1.52	1595.95
1.69	1522.15
1.85	1486.54
2.02	1417.81
2.17	1384.64
2.35	1320.62
2.50	1289.72
2.69	1259.55
2.85	1227.85
3.02	1199.13
3.19	1171.08
3.35	1116.93
3.52	1116.93
3.69	1090.80
3.86	1065.28
4.02	1040.36
4.19	1016.03
4.34	992.26
4.52	992.26
4.69	992.26
4.86	967.28
5.02	944.65
5.19	922.56
5.36	900.98

5.51	900.98
5.69	900.98
5.86	879.90

Stenner et al., 1997

TCE Oral Gavage 100.0 mg/kg

Hours	CBldTCA	CTCOG	CTCOH
0.251	0.727	0.412	2.02
0.439	1.64	0.727	2.77
0.966	2.11	0.791	2.93
1.43	2.46	0.886	3.12
2.42	3.34	0.668	2.4
3.41	3.97	0.166	2.43
4.47	4.07	0.105	2.28
5.41	4.07	nan	1.96
6.66	nan	0.0462	nan
8.4	4.61	nan	0.364
16.8	3.77	nan	nan

TCOH IV 100.0 mg/kg without bile cannulation

Hours	AUrnTCOGTCOH	CBldTCA	TotCTCOH	zAUrnTCA
0.534	nan	2.04	nan	nan
0.979	nan	3.7	72.8	nan
2.05	nan	5.21	41.3	nan
3.03	nan	5.5	27.5	nan
4.99	nan	6.47	14.3	nan
8.01	nan	7.1	6.89	nan
11.0	nan	5.4	1.97	nan
16.0	nan	4.57	nan	nan
24.0	nan	2.63	nan	nan
48.0	7.9	nan	nan	0.46

TCOH IV 5.0 mg/kg with bile cannulation

Hours	AUrnTCOGTCOH	zAUrnTCA
48.0	0.5	0.01

TCOH IV 20.0 mg/kg with bile cannulation

Hours	AUrnTCOGTCOH	zAUrnTCA
48.0	3.1	0.03

TCOH IV 100.0 mg/kg with bile cannulation

Hours	AUrnTCOGTCOH	CBldTCA	TotCTCOH	zAUrnTCA
0.534	nan	0.389	nan	nan
1.07	nan	0.973	45.7	nan
2.05	nan	1.65	9.84	nan
3.03	nan	2.38	2.95	nan
4.99	nan	1.99	0.984	nan
8.01	nan	1.8	nan	nan
11.0	nan	1.17	nan	nan
16.0	nan	0.827	nan	nan
24.0	nan	0.584	nan	nan
48.0	8.1	nan	nan	0.09

Templin et al., 1995

Data were truncated in EPA (2011) file so they were digitized

TCE Oral Gavage 100.0 mg/kg

Hours	CBldTCA	CTCOH	CVen
0.25	0.94	0.779	6.377
0.5	1.39	1.386	10.362
0.75	1.91	1.716	11.644
1.0	1.63	1.750	7.695
1.5	2.22	1.783	2.645
2.0	4.26	2.357	1.771
2.5	3.80	2.880	1.062
3.0	5.01	2.33	nan
4.0	6.05	2.180	nan
5.0	6.75	1.953	nan
6.0	7.11	1.819	nan
9.0	7.64	0.893	nan
12.0	7.30	nan	nan
24.0	4.46	nan	nan
48.0	1.52	nan	nan

Yu et al., 2000

TCA IV 1.0 mg/kg

Hours	CBldTCA	CLivTCA	CPlasTCA	zAUrnTCA
0.083	3.42323	1.86276	4.67324	nan
0.5	2.58360	1.03432	3.4314	nan
1.0	2.27240	0.9804	2.97388	nan
3.0	2.01431	1.24511	2.82682	nan
6.0	1.66243	1.36766	2.27126	0.06622
9.0	1.21006	1.09968	1.66668	0.07522
24.0	0.32304	0.54576	0.45098	0.10179

TCA IV 10.0 mg/kg

Hours	CBldTCA	CLivTCA	CPlasTCA	zAUrnTCA
0.083	35.35159	18.3008	46.8958	nan
0.5	29.26494	14.6243	38.2356	nan
1.0	25.21099	14.10142	34.314	nan
3.0	21.34739	15.78444	29.5754	nan
6.0	13.80485	11.7648	17.974	0.76290
9.0	10.84077	9.10138	13.33344	0.91934
24.0	3.036544	5.89874	4.31376	1.43580

TCA IV 50.0 mg/kg

Hours	CBldTCA	CLivTCA	CPlasTCA	zAUrnTCA
0.083	143.30997	78.9222	176.472	nan
0.5	103.89789	69.2816	130.8834	nan
1.0	104.38809	68.1378	128.4324	nan
3.0	70.13945	57.6802	90.3602	nan
6.0	42.68825	44.4448	57.0266	6.40705
9.0	35.05747	45.4252	48.3664	6.27805
24.0	8.81216	20.2616	12.8269	9.08382

APPENDIX J. DATA FOR HUMAN VALIDATION FIGURES

The following data are for generating human validation figures in Appendix C.

Bernauer et al., 1996

```
TCE Inhalation 40.0 ppm for 6 hours
Hours, zAUrnTCA, AUrnTCOGTCOH, zAUrnNDCVC
   6.0    1.557452405   13.63675325   0.005309749
  11.0    3.14839841    33.61944879   0.012434097
  16.0    5.681351918   51.78263372   0.019694974
  23.0    8.719500561   61.25685742   0.025776734
  30.0   11.70391989    71.08859899   0.035646562
  35.0   14.45667515    81.97374145   0.042820557
  40.0   16.84309415    91.93316798   0.05376152
  47.0   19.6760945     98.27911027   0.060468832
```

```
TCE Inhalation 80.0 ppm for 6 hours
Hours, zAUrnTCA, AUrnTCOGTCOH, zAUrnNDCVC
   6.0    1.941365664    36.6438435    0.007553303
  11.0    4.874486405    86.08691135   0.013224905
  16.0    7.841594641   124.9572477    0.027986974
  23.0   11.14857782    151.426392     0.036437397
  30.0   16.28748693    174.630428     0.057308365
  35.0   21.28364856    192.4174939    0.068022128
  40.0   27.26544753    208.1833023    0.078623254
  47.0   31.66206976    220.8519223    0.088400143
```

```
TCE Inhalation 160.0 ppm for 6 hours
Hours, zAUrnTCA, AUrnTCOGTCOH, zAUrnNDCVC
   6.0    2.838297949    62.99517723   0.01122279
  11.0    8.369594126   150.9920375    0.026161736
  16.0   16.2537551     229.5471746    0.053723225
  23.0   24.5176767     284.5357705    0.064310553
  30.0   35.0353951     305.7381042    0.073536529
  35.0   44.90091589    334.9696792    0.078057851
  40.0   55.13794165    359.5181595    0.091739498
  47.0   63.40186326    375.6974964    0.102725693
```

Chiu et al., 2007

```
Data were truncated in EPA (2011) file -- data for CAlvPPM were digitized
   from the figures in EPA (2011) because they were easier to see than in the
   Chiu et al., (2007) -- missing points for AUrnTCOGTCOH_Coll data only were
   digitized from Chiu et al., (2007)
```

```
TCE Inhalation -- Experiment A-TRI–1
Hours, CAlvPPM
    0.33651    0.27033
    0.67837    0.40502
    1.03052    0.39808
    1.36755    0.5123
    1.70588    0.5123
    2.03845    0.50352
    2.77083    0.48811
    3.07712    0.42657
    3.74737    0.42657
    4.05778    0.49661
    4.44976    0.32579
    4.76388    0.45551
    5.25717    0.27504
    5.45332    0.37279
    5.98011    0.37928
    6.018      0.26662
    6.24254    0.15024
```

6.2821	0.09554
6.47547	0.12084
6.55778	0.06928
6.59933	0.05573
7.05628	0.06055
7.10099	0.04483
7.64078	0.04055
8.28416	0.0257
9.36403	0.01903
10.07585	0.01807
11.04917	0.01552
14.66279	0.01129
16.0792	0.00659
23.25178	0.00728
27.64488	0.00385
47.77045	0.00148
48.31664	0.002
52.71695	0.000767705
60.3463	0.000440129
74.331	0.000692107
76.61899	0.000232247
97.40265	0.000304092
106.81168	0.000142676

Hours,	CVen,	CBldTCA,	TotCTCOH,	CTCOH,	zAUrnTCA_Coll,	AUrnTCOGTCOH_Coll
1.0	0.0045	0.002	0.007	0.005	nan	nan
2.0	0.0045	0.004	0.048	0.007	nan	nan
4.0	0.005	0.01	0.066	0.011	nan	nan
5.75	0.004	0.019	0.0995	0.027	nan	nan
6.0	0.002	0.0265	0.088	0.0165	nan	nan
7.0	0.002	0.0275	0.104	0.0195	nan	nan
8.0	0.001	0.0375	0.037	0.02	nan	nan
23.0	nan	nan	nan	nan	nan	0.5003
30.0	nan	nan	nan	nan	nan	0.6866
31.0	nan	nan	nan	nan	0.0101	0.7662
36.0	nan	nan	nan	nan	nan	1.0048
39.0	nan	nan	nan	nan	0.0165	1.0342
39.5	nan	nan	nan	nan	0.0277	1.0736
41.0	nan	0.047	0.0035	0.002	nan	nan
46.0	nan	nan	nan	nan	nan	1.1472
76.0	nan	nan	nan	nan	nan	1.1793
78.0	nan	nan	0.0015	nan	nan	nan
95.0	nan	nan	nan	nan	nan	1.1995
98.0	nan	0.024	0.003	nan	nan	nan
122.0	nan	0.0175	nan	nan	0.0465	1.2039

TCE Inhalation -- Experiment A-TRI–2

Hours,	CAlvPPM
0.33287	0.26742
0.66683	0.38904
1.00046	0.38904
1.01848	0.33857
1.33583	0.30729
1.33583	0.37183
1.68463	0.38904
1.69468	0.30334
1.9923	0.34856
2.3283	0.36587
2.38437	0.43422
2.67603	0.42178
2.69199	0.23576
3.00694	0.4413
3.43143	0.52543
3.59439	0.42865
3.70291	0.47843
4.08235	0.39538
4.55996	0.39538
4.6642	0.47843
5.24097	0.4413

5.68258	0.59601
5.84717	0.47076
6.05242	0.1774
6.23514	0.13567
6.27234	0.11068
6.53125	0.03514
6.83329	0.0639
7.08158	0.04886
7.49774	0.03689
7.94781	0.02611
30.63063	0.00427
34.78885	0.00128
34.99641	0.00207
39.04429	0.00302
47.00659	0.0018
50.96741	0.00102
55.26197	0.000357251
55.59168	0.000465644
70.86166	0.000181239
77.75206	0.00019969
78.21594	0.000295237
85.82145	0.000628888
85.82145	0.00088867
88.30718	0.000367793
95.74804	0.000226511
96.89394	0.000093746
97.47203	0.000162381

Hours, CVen, CBldTCA, TotCTCOH, CTCOH, zAUrnTCA_Coll, AUrnTCOGTCOH_Coll

1.0	0.003	0.001	0.007	nan	nan	nan
2.0	0.003	0.002	0.011	nan	nan	nan
4.0	nan	nan	0.041	nan	nan	nan
5.75	0.006	0.0105	0.057	0.0025	nan	nan
6.0	0.0015	0.0115	0.0595	0.003	0.017	nan
8.0	0.0005	0.0125	0.044	0.0025	nan	nan
14.0	nan	nan	nan	nan	0.0336	0.5175
24.0	nan	0.0205	0.01	nan	nan	0.9178
32.0	nan	nan	nan	nan	0.039	0.9796
37.0	nan	nan	nan	nan	nan	1.0985
39.0	nan	nan	nan	nan	nan	1.1677
42.0	nan	nan	nan	nan	0.0491	1.2565
48.0	nan	nan	nan	nan	nan	1.3254
70.0	nan	nan	nan	nan	0.062	1.3535
74.0	nan	0.0325	nan	nan	nan	nan
97.0	nan	nan	nan	nan	0.0709	1.3605
99.0	nan	0.024	nan	nan	nan	nan
121.0	nan	nan	nan	nan	0.0847	1.365
123.0	0.001	0.0285	nan	0.0055	nan	nan
123.0	nan	0.024	nan	nan	nan	nan
142.5	nan	nan	nan	nan	0.0962	1.36

TCE Inhalation -- Experiment B-TRI–1
Hours, CAlvPPM

0.33747	0.28443
0.6653	0.27973
1.0077	0.2892
1.36635	0.29405
1.36635	0.37493
1.65847	0.37995
2.34266	0.39281
2.37103	0.3393
2.72624	0.28443
2.72624	0.33481
3.23431	0.28443
3.32909	0.37493
3.92108	0.3393
4.30698	0.2892
4.51394	0.36265
5.13429	0.30808

5.13429	0.36265
5.80485	0.36265
6.04729	0.2345
6.15745	0.16644
6.29986	0.13495
6.37614	0.08726
6.45333	0.10238
6.87836	0.06731
6.91987	0.04956
7.3845	0.05458
7.64678	0.03576
8.1504	0.04352
9.11561	0.02633
10.00069	0.02391
10.86659	0.01784
14.38372	0.01134
24.22034	0.00623
26.60401	0.00505
38.68052	0.00396
47.23379	0.00282
64.04482	0.0024
73.28603	0.00185
79.05846	0.0016
83.86068	0.00127
92.55842	0.00114
94.24444	0.000953537
107.19626	0.000604378

Hours, CVen, CBldTCA, TotCTCOH, CTCOH, AUrnTCOGTCOH_Coll

1.0	0.002	0.002	0.0055	0.003	nan
2.0	0.0045	0.005	0.011	0.006	nan
4.0	0.003	0.12	0.034	0.008	nan
6.0	0.004	0.031	0.053	0.011	nan
6.5	nan	nan	nan	nan	0.6936
7.0	0.001	0.035	0.04	0.026	nan
8.0	0.001	0.0425	0.04	0.0135	nan
20.5	nan	nan	nan	nan	1.1404
23.0	nan	nan	nan	nan	1.3606
26.5	nan	0.0725	0.007	0.0055	1.4823
29.5	nan	nan	nan	nan	1.6973
30.5	nan	nan	nan	nan	1.8812
39.5	nan	nan	nan	nan	2.0137
48.0	nan	0.0685	0.0025	0.0025	2.1577
72.0	nan	0.0485	0.001	nan	2.1792
91.5	nan	nan	nan	nan	2.2126
98.5	nan	nan	0.0015	nan	nan
116.5	nan	nan	nan	nan	2.23

TCE Inhalation -- Experiment B-TRI–2
Hours, CAlvPPM

0.33771	0.21519
0.33972	0.29201
0.6828	0.2292
1.00551	0.24902
1.01149	0.18596
1.33383	0.07176
1.67135	0.079
1.69131	0.0457
1.69131	0.05822
2.33598	0.2292
2.68408	0.26966
2.71614	0.34356
3.32358	0.37204
3.37928	0.26522
3.99509	0.39102
4.33614	0.31726
4.64525	0.41098
5.12631	0.48193
5.18137	0.37826

5.752	0.33235
6.12557	0.15597
6.3101	0.10579
6.41586	0.07418
6.57003	0.05726
7.08029	0.04724
7.5044	0.0347
7.99178	0.03258
11.16981	0.02959
14.31557	0.01909
24.22282	0.00853
25.79598	0.00923
35.04127	0.00637
40.7439	0.0068
49.8559	0.00387
53.72793	0.00534
62.76901	0.0034
72.98405	0.00329
76.89797	0.00267
85.77311	0.00238
97.97148	0.000935553

Hours, CVen, CBldTCA, TotCTCOH, CTCOH, AUrnTCOGTCOH_Coll

1.0	0.0025	0.002	nan	nan	nan
5.75	0.006	0.041	0.0425	0.011	nan
6.0	0.003	0.034	0.037	0.0075	nan
7.0	0.001	0.0325	0.036	0.0065	nan
8.0	0.001	0.042	0.0325	0.008	nan
15.0	nan	nan	nan	nan	0.2776
26.5	nan	0.057	0.011	nan	0.8985
32.0	nan	nan	nan	nan	1.1068
36.0	nan	nan	nan	nan	1.3213
42.0	nan	nan	nan	nan	1.4584
50.0	nan	0.06	0.004	nan	1.6555
74.0	nan	0.068	0.0025	nan	1.7119
95.0	nan	nan	nan	nan	1.7378
100.0	nan	nan	0.001	nan	nan
118.0	nan	nan	nan	nan	1.7532
145.0	nan	0.0405	nan	nan	nan

TCE Inhalation -- Experiment C-TRI–1

Hours, CAlvPPM

0.33719	0.42754
0.33919	0.3267
0.66955	0.3589
1.01963	0.42754
1.03056	0.36476
1.35177	0.31221
1.68303	0.30719
2.02229	0.38918
2.33677	0.44738
2.63692	0.48514
3.0111	0.39554
3.41806	0.3267
3.94492	0.33204
4.45692	0.29262
4.55838	0.22726
5.05929	0.21025
5.11352	0.29262
5.80463	0.29262
5.87381	0.21368
6.15158	0.07429
6.15158	0.11032
6.66768	0.05003
7.4797	0.02501
8.40056	0.03272
9.25763	0.02313
10.33597	0.01739
11.59473	0.01291

```
   14.18178   0.01942
   23.54776   0.00709
   27.66469   0.00756
   33.28071   0.00354
   38.63878   0.00312
   45.93511   0.00328
   52.76487   0.00131
   63.10139   0.00354
   71.62979   0.00149
   76.27176   0.000635873
   81.31083   0.000307679
   86.58019   0.00116
   93.84402   0.000371305
   97.12431   0.000698533
  105.89822   0.000470409
  107.16031   0.00037737


Hours, CVen, CBldTCA, TotCTCOH, CTCOH, zAUrnTCA_Coll, AUrnTCOGTCOH_Coll
    1.0    0.001    0.001   0.005    0.003    nan      nan
    2.0    0.004    0.004   0.0165   0.006    nan      nan
    4.0    0.004    0.014   0.213    0.02     nan      nan
    5.75   nan      nan     0.094    nan      nan      nan
    6.0    0.0025   0.015   0.095    0.016    nan      nan
    7.0    0.001    0.035   0.088    0.024    0.0106   0.5381
    8.0    nan      nan     0.075    nan      nan      nan
   28.0    nan      0.055   0.012    0.006    0.0213   0.9118
   38.0    nan      nan     nan      nan      nan      1.1632
   46.0    nan      nan     nan      nan      0.0333   1.3584
   52.0    0.0005   0.053   0.014    0.0015   nan      nan
   70.0    nan      nan     nan      nan      0.0527   1.4847
   75.0    nan      0.045   0.012    0.001    nan      nan
   95.0    nan      nan     nan      nan      0.067    1.5212
   99.0    nan      0.033   nan      nan      nan      nan
  118.0    nan      nan     nan      nan      0.0823   1.5427
  121.0    nan      0.027   0.001    nan      nan      nan
  141.0    nan      nan     nan      nan      0.0951   1.5485


TCE Inhalation -- Experiment C-TRI–2
Hours, CAlvPPM
    0.37754   0.25017
    0.66345   0.27139
    0.95792   0.2944
    1.36798   0.32046
    1.66496   0.33152
    2.00184   0.22983
    2.33456   0.23776
    2.37768   0.31507
    2.7259    0.31507
    3.41212   0.36579
    3.77583   0.27603
    3.86911   0.32046
    4.53981   0.24182
    5.35936   0.29044
    5.75243   0.22673
    5.93062   0.28075
    6.03281   0.10426
    6.06973   0.07503
    6.18186   0.05567
    6.32686   0.0442
    6.48318   0.04006
    6.87427   0.02604
    7.00126   0.03279
    7.56073   0.01089
    8.16492   0.000339867
    9.09053   0.01669
   10.35847   0.01123
   22.67436   0.00462
   28.2442    0.00183
   28.2442    0.00246
```

33.7524	0.000658552
34.37591	0.00119
34.75553	0.00242
37.76258	0.00192
47.03877	0.00242
53.59972	0.000915154
54.2578	0.00136
71.31404	0.000224685
71.75049	0.000636587
75.61596	0.000362494
75.61596	0.00108
82.66109	0.000181451
83.16699	0.000132807
85.7433	0.000775007
88.83196	0.000625881
95.93062	0.000667549
112.55973	0.000625881

Hours, CVen, CBldTCA, TotCTCOH, CTCOH, zAUrnTCA_Coll, AUrnTCOGTCOH_Coll

Hours	CVen	CBldTCA	TotCTCOH	CTCOH	zAUrnTCA_Coll	AUrnTCOGTCOH_Coll
1.0	0.002	0.001	0.006	nan	nan	nan
2.0	0.002	0.004	0.013	nan	nan	nan
4.0	0.003	0.0065	0.055	0.002	nan	nan
5.75	0.003	0.012	0.097	0.003	nan	nan
6.0	0.001	0.0135	0.066	0.004	nan	nan
7.0	0.0005	0.018	0.069	0.003	nan	nan
8.0	0.001	0.0155	0.079	0.003	0.0133	nan
22.0	nan	nan	nan	nan	nan	0.5968
26.0	nan	0.048	0.013	0.002	nan	nan
29.0	nan	nan	nan	nan	0.0232	0.9005
33.5	nan	nan	nan	nan	nan	1.0882
37.5	nan	nan	nan	nan	0.0315	1.2845
46.0	nan	nan	nan	nan	nan	1.556
51.0	nan	nan	nan	nan	0.0454	1.6346
53.0	nan	0.058	0.0095	nan	nan	nan
70.0	nan	nan	nan	nan	nan	1.6844
75.0	nan	0.051	0.004	nan	nan	nan
94.0	nan	nan	nan	nan	0.0542	1.706
98.0	nan	0.038	nan	nan	nan	nan
124.0	nan	0.036	nan	nan	nan	nan
142.0	nan	nan	nan	nan	0.0575	1.7109

TCE Inhalation -- Experiment D-TRI–1
Hours, CAlvPPM

Hours	CAlvPPM
0.3378	0.3334
0.68032	0.39061
1.01775	0.39697
1.33927	0.34435
1.67983	0.28922
2.0497	0.46358
2.42716	0.36029
2.72647	0.38435
3.04802	0.43597
3.46518	0.29871
4.10331	0.3334
4.94712	0.31355
5.15293	0.47113
5.52396	0.33884
5.85816	0.42211
5.99312	0.66574
6.20514	0.16697
6.24244	0.07966
6.24244	0.23978
6.35571	0.11112
6.65991	0.06211
7.18238	0.08096
7.61691	0.05388
7.65353	0.03813
7.98148	0.03012
8.21445	0.05133

```
     9.22741   0.00911
     9.28288   0.01373
    11.31323   0.01172
    23.19762   0.00731
    27.30542   0.00616
    27.30542   0.01351
    74.47583   0.000933536
    76.6497    0.00183
    82.76195   0.000680134
   103.31113   0.00045265


Hours, CVen, CBldTCA, TotCTCOH, CTCOH, zAUrnTCA_Coll, AUrnTCOGTCOH_Coll
    1.0    0.004    0.003    0.006    0.0025   nan      nan
    2.0    nan      nan      0.011    nan      nan      nan
    4.0    0.0035   0.032    0.035    0.016    nan      nan
    5.75   0.007    0.056    0.073    0.022    nan      nan
    6.0    0.0025   0.047    0.104    0.014    0.0141   nan
    7.0    nan      nan      0.366    nan      nan      nan
    8.0    0.001    0.072    0.133    0.0095   nan      nan
   25.0    nan      0.0595   0.01     0.005    nan      0.2368
   31.0    nan      nan      nan      nan      nan      0.3721
   33.0    nan      nan      nan      nan      nan      0.3835
   35.0    nan      nan      nan      nan      nan      0.4405
   40.0    nan      nan      nan      nan      0.0171   0.4633
   48.0    nan      nan      nan      nan      nan      0.6079
   50.0    nan      0.0875   nan      0.003    nan      nan
   72.0    nan      nan      nan      nan      nan      0.6947
   74.0    nan      0.052    0.0025   nan      nan      nan
   94.0    nan      nan      nan      nan      nan      0.7139
  100.0    nan      nan      0.001    nan      nan      nan
  118.0    nan      nan      nan      nan      nan      0.728
  132.0    nan      nan      nan      nan      nan      0.7312


TCE Inhalation -- Experiment F-TRI–1
Hours, CAlvPPM
     0.33837   0.21929
     0.34042   0.45748
     0.68599   0.17757
     1.00554   0.45149
     1.34116   0.20871
     1.3493    0.33777
     1.67768   0.67286
     1.68787   0.30697
     2.01405   0.56497
     2.03611   0.31207
     2.36004   0.40896
     2.67009   0.48867
     2.95221   0.30195
     2.97013   0.39051
     3.36034   0.26993
     3.7109    0.52891
     4.07824   0.37785
     4.35365   0.49679
     4.75575   0.27441
     4.83701   0.39051
     4.95551   0.52891
     5.38055   0.34339
     5.64058   0.41576
     6.12438   0.29701
     6.16155   0.07362
     6.16155   0.1419
     6.22902   0.09971
     6.53005   0.05981
     6.73063   0.05089
     7.01334   0.03935
     7.43279   0.04203
     7.74499   0.03093
     8.21814   0.0236
     8.35856   0.03093
```

9.13056	0.01766
9.24173	0.02472
10.0344	0.01911
11.22972	0.01605
15.06886	0.00506
28.79097	0.0035
36.18992	0.00466
49.45187	0.00238
51.52902	0.0016
59.72697	0.00184
73.81488	0.000985962
83.00868	0.000627576
98.45274	0.000570343
102.58808	0.000358273

Hours,	CVen,	CBldTCA,	TotCTCOH,	CTCOH,	zAUrnTCA_Coll,	AUrnTCOGTCOH_Coll
1.0	0.0025	0.002	0.014	0.002	nan	nan
2.0	nan	nan	0.0115	nan	nan	nan
4.0	0.004	0.018	0.022	0.008	nan	nan
5.75	0.005	0.029	0.05	0.0095	nan	nan
6.0	0.002	0.0445	0.05	0.0175	nan	0.0063
7.0	0.001	0.041	0.141	0.01	nan	nan
8.0	0.001	0.048	0.044	0.01	nan	0.2254
12.0	nan	nan	nan	nan	nan	0.4775
14.0	nan	nan	nan	nan	nan	0.6152
24.0	nan	nan	nan	nan	nan	0.9452
26.0	nan	0.067	0.0075	0.003	nan	nan
30.0	nan	nan	nan	nan	nan	1.0952
32.0	nan	nan	nan	nan	0.0088	1.143
36.0	nan	nan	nan	nan	nan	1.2548
39.0	nan	nan	nan	nan	nan	1.3098
42.0	nan	nan	nan	nan	nan	1.3584
48.0	nan	nan	nan	nan	nan	1.37
50.0	0.0005	0.073	nan	0.001	nan	nan
72.0	nan	nan	nan	nan	nan	1.36798
74.0	nan	0.07	0.003	0.001	nan	nan
98.0	nan	nan	nan	nan	nan	1.38525
101.0	nan	0.0505	nan	nan	nan	nan
123.0	nan	0.039	0.001	nan	nan	1.38525
143.0	nan	nan	nan	nan	nan	1.36798

TCE Inhalation -- Experiment F-TRI–2

Hours,	CAlvPPM
0.32906	0.43062
0.33107	0.34408
0.66266	0.42358
0.66589	0.29272
1.00243	0.54789
1.01471	0.37863
1.34751	0.32318
1.35574	0.40446
1.67765	0.07371
2.01622	0.05605
2.31075	0.48975
2.32486	0.15691
2.68075	0.33292
3.03519	0.53011
3.35791	0.52316
3.68791	0.41802
4.03067	0.557
4.13001	0.33292
4.54141	0.54789
4.59145	0.33292
5.04881	0.33292
5.07964	0.53892
5.68858	0.33845
5.75125	0.46764
6.0309	0.18143
6.06772	0.10018

6.10477	0.07132
6.14204	0.05532
6.24762	0.13797
6.44069	0.04479
6.55141	0.06087
6.86997	0.04706
7.03929	0.03699
7.64683	0.03055
8.06761	0.01508
16.30584	0.01008
23.15333	0.00767
27.96176	0.00521
34.39112	0.00284
36.06337	0.00633
40.14147	0.00323
49.6728	0.00144
53.04804	0.00181
59.33504	0.00157
59.69732	0.00223
73.87206	0.00152
76.5267	0.000892128
83.63908	0.00115
94.69746	0.000851859
100.51837	0.00030938
101.1321	0.000224652
102.37082	0.000560273

Hours,	CVen,	CBldTCA,	TotCTCOH,	CTCOH,	zAUrnTCA_Coll,	AUrnTCOGTCOH_Coll
1.0	0.0035	0.002	0.0065	nan	nan	nan
2.0	0.001	0.0035	0.018	nan	nan	nan
4.0	0.005	0.02	0.038	0.008	nan	nan
5.75	0.006	0.039	0.065	0.009	nan	nan
6.0	0.002	0.0425	0.043	0.009	nan	0.5917
7.0	nan	nan	0.041	nan	nan	nan
8.0	0.001	0.048	0.036	0.007	nan	nan
9.5	nan	nan	nan	nan	nan	1.0628
15.5	nan	nan	nan	nan	nan	1.4811
23.0	nan	nan	nan	nan	nan	1.9016
26.5	nan	0.074	0.012	0.002	nan	2.0542
30.0	nan	nan	nan	nan	nan	2.1926
34.0	nan	nan	nan	nan	nan	2.3728
39.0	nan	nan	nan	nan	nan	2.4387
41.0	nan	nan	nan	nan	0.0198	2.4618
48.0	nan	nan	nan	nan	nan	2.5126
50.5	nan	nan	0.0025	nan	nan	nan
72.0	nan	nan	nan	nan	nan	2.59834
74.0	nan	0.067	0.001	nan	nan	nan
94.0	nan	0.0545	nan	nan	nan	2.59834
118.0	nan	nan	nan	nan	0.024	nan
120.0	nan	nan	nan	nan	nan	2.53018
128.0	nan	0.036	nan	nan	nan	nan
146.0	nan	nan	nan	nan	nan	2.59834

TCE Inhalation -- Experiment G-TRI–1

Hours,	CAlvPPM
0.33359	0.31868
0.66834	0.34502
1.00588	0.26303
1.00588	0.36138
1.33263	0.10765
1.66734	0.05517
2.00328	0.58389
2.01525	0.4586
2.42128	0.29435
2.63825	0.41802
2.99354	0.58389
3.4374	0.35545
3.92363	0.38483
4.32648	0.41802

5.19817	0.52176
5.82833	0.39778
6.14214	0.10109
6.28282	0.07237
6.42673	0.05338
6.65275	0.03051
7.00261	0.0525
7.04447	0.02334
7.42376	0.01721
9.38855	0.04069
10.78064	0.02865
12.79924	0.02647
24.50735	0.01138
26.70338	0.00621
27.47828	0.00802
32.66231	0.00361
37.9098	0.00601
48.00026	0.00113
48.51793	0.00231
51.37465	0.00173
58.36279	0.00323
72.58779	0.00143
72.58779	0.00328
81.8738	0.000369405
83.74908	0.000462617
85.25986	0.0002084
86.17937	0.00106
96.74179	0.0005246
102.4379	0.000264462

Hours,	CVen,	CBldTCA,	TotCTCOH,	CTCOH,	zAUrnTCA_Coll,	AUrnTCOGTCOH_Coll
1.0	0.002	0.001	0.008	nan	nan	nan
2.0	0.004	0.002	nan	nan	nan	nan
4.0	0.004	0.0135	0.024	0.008	nan	nan
5.75	0.005	0.0255	0.0455	0.011	nan	nan
6.0	0.001	0.027	0.049	0.013	nan	nan
7.0	nan	nan	0.049	nan	nan	nan
8.0	nan	nan	0.041	nan	nan	nan
13.0	nan	nan	nan	nan	0.0037	nan
24.0	nan	nan	nan	nan	nan	0.778
27.0	nan	nan	0.009	nan	nan	nan
30.0	nan	nan	nan	nan	nan	0.9906
51.0	nan	0.0665	0.006	nan	nan	nan
72.0	nan	0.0635	nan	nan	nan	1.0389
96.0	nan	0.0445	nan	nan	nan	1.0529
144.0	nan	0.0385	nan	nan	nan	nan

Fisher et al., 1998

TCE Inhalation 105.5 ppm for 4 hours -- Male subject 1

Hours,	CVen,	CTCOH,	CBldTCA,	zAUrntTCA,	AUrnTCOGTCOH,	TotCTCOH,	CDCVG_Mole
0.5	1.98	nan	0.15	nan	nan	nan	0.00886
1.0	2.69	0.39	0.50	nan	nan	0.39	0.0349
2.0	3.38	1.30	1.07	nan	nan	1.30	0.0461
3.0	3.76	2.18	2.11	nan	nan	2.18	0.0337
4.0	3.95	2.83	3.12	nan	nan	2.83	0.0313
4.25	3.26	2.94	2.87	nan	nan	2.94	0.0241
4.5	2.54	3.21	3.39	1.47	13.94	3.21	0.0132
5.0	1.12	2.78	4.00	nan	nan	2.78	0.00552
6.0	0.72	2.84	4.09	2.82	23.22	2.84	0.00417
8.0	0.52	2.52	4.76	5.02	30.95	2.52	0.000671
10.0	0.31	2.03	5.52	7.10	37.58	2.03	nan
11.5	nan	nan	nan	8.87	43.49	nan	nan
12.0	0.28	1.56	6.16	10.22	46.17	1.56	nan
14.0	0.23	1.56	6.48	12.67	50.32	1.56	nan
16.0	0.17	1.31	8.12	15.33	56.69	1.31	nan
18.0	0.15	1.21	7.18	16.85	61.37	1.21	nan
20.0	nan	1.15	8.56	nan	nan	1.15	nan
20.25	nan	nan	nan	22.83	65.35	nan	nan

22.0	nan	nan	8.14	25.23	68.94	nan	nan
26.0	nan	nan	nan	30.03	74.63	nan	nan
31.5	nan	nan	nan	33.10	79.76	nan	nan
34.25	nan	nan	nan	39.59	82.89	nan	nan
35.5	nan	nan	nan	42.21	84.29	nan	nan
36.75	nan	nan	nan	48.47	86.91	nan	nan
44.75	nan	nan	nan	52.39	90.23	nan	nan
46.0	nan	nan	9.30	nan	nan	nan	nan
52.0	nan	nan	nan	55.28	91.80	nan	nan
54.0	nan	nan	nan	nan	nan	nan	nan
54.5	nan	nan	nan	58.64	93.75	nan	nan
56.5	nan	nan	nan	59.80	94.88	nan	nan
59.5	nan	nan	nan	62.40	96.10	nan	nan
60.5	nan	nan	nan	65.00	96.99	nan	nan
68.5	nan	nan	nan	79.17	99.59	nan	nan
69.75	nan	nan	7.37	nan	nan	nan	nan
70.25	nan	nan	nan	83.51	100.64	nan	nan
73.0	nan	nan	nan	88.15	102.16	nan	nan
79.5	nan	nan	nan	99.19	104.07	nan	nan
81.5	nan	nan	nan	100.11	104.74	nan	nan
84.75	nan	nan	nan	100.62	104.94	nan	nan
93.75	nan	nan	6.97	nan	nan	nan	nan

TCE Inhalation 49.3 ppm for 4 hours -- Male subject 2

Hours,	CVen,	CTCOH,	CBldTCA,	zAUrntTCA,	AUrnTCOGTCOH,	TotCTCOH
0.5	0.61	0.44	0.29	nan	nan	0.44
1.0	0.74	0.55	0.65	nan	nan	0.55
2.0	1.11	0.83	1.47	nan	nan	0.83
3.0	1.01	1.08	2.27	nan	nan	1.08
4.0	1.05	1.35	2.91	nan	nan	1.35
4.25	0.81	1.26	2.99	nan	nan	1.26
4.5	0.46	1.34	3.12	0.041	8.45	1.34
5.0	nan	1.11	3.49	0.062	15.20	1.11
6.0	nan	1.01	3.66	0.15	21.60	1.01
8.0	nan	0.90	4.29	0.26	28.09	0.90
10.0	nan	0.76	4.69	0.41	35.67	0.76
12.0	nan	nan	5.11	0.53	39.98	nan
14.0	nan	0.66	5.17	0.65	43.78	0.66
16.0	nan	0.63	5.26	0.80	47.68	0.63
18.0	nan	0.56	5.66	0.92	50.54	0.56
20.0	nan	0.51	5.18	1.05	53.03	0.51
22.0	nan	nan	5.69	1.18	55.30	nan
31.25	nan	nan	nan	1.46	60.62	nan
49.0	nan	nan	6.67	2.20	69.80	nan
64.25	nan	nan	nan	3.61	73.15	nan
71.75	nan	nan	6.49	4.36	74.82	nan
77.0	nan	nan	nan	5.03	76.02	nan
97.5	nan	nan	6.01	nan	nan	nan

TCE Inhalation 55.2 ppm for 4 hours -- Male subject 3

Hours,	CVen,	CTCOH,	CBldTCA,	zAUrntTCA,	AUrnTCOGTCOH,	TotCTCOH
0.5	1.89	0.63	0.43	0.002	0.0	0.63
1.0	1.36	1.07	0.55	nan	nan	1.07
2.0	2.68	1.57	1.07	nan	nan	1.57
3.0	2.67	1.90	1.57	0.082	8.24	1.90
4.0	2.79	1.94	1.96	nan	nan	1.94
4.25	2.42	2.02	2.01	nan	nan	2.02
4.5	1.52	2.26	2.19	0.184	11.60	2.26
5.0	0.82	1.02	2.28	nan	nan	1.02
5.5	nan	nan	nan	0.249	13.64	nan
6.0	0.37	0.96	2.52	nan	nan	0.96
6.5	nan	nan	nan	0.307	15.64	nan
8.0	0.29	1.65	2.92	0.539	19.73	1.65
10.0	nan	1.38	3.20	0.852	23.26	1.38
12.0	nan	1.26	3.56	1.35	28.95	1.26
14.0	nan	1.13	4.19	1.78	28.95	1.13
16.0	nan	1.03	3.90	2.12	29.79	1.03
18.0	nan	1.05	4.95	2.48	32.07	1.05
20.0	nan	0.90	5.04	2.89	34.21	0.90

```
  22.0    nan    nan    5.08    3.48    38.49   nan
  24.0    nan    nan    nan     4.28    43.06   nan
  33.0    nan    nan    nan     5.35    47.48   nan
  34.0    nan    nan    nan     5.66    48.60   nan
  40.0    nan    nan    nan     6.72    52.15   nan
  44.25   nan    nan    nan     7.42    53.88   nan
  44.75   nan    nan    5.51    nan      nan    nan
  47.25   nan    nan    nan     8.14    55.21   nan
  52.0    nan    nan    nan     8.93    57.21   nan
  59.0    nan    nan    nan    10.17    59.15   nan
  67.75   nan    nan    nan    11.19    60.89   nan
  68.75   nan    nan    9.45    nan      nan    nan
  72.25   nan    nan    nan    12.56    61.46   nan
  77.0    nan    nan    nan    13.78    61.84   nan
  83.0    nan    nan    nan    14.44    62.20   nan
  92.0    nan    nan    nan    15.63    62.56   nan
  93.0    nan    nan    4.27    nan      nan    nan
```

```
TCE Inhalation 101.5 ppm for 4 hours -- Male subject 3
Hours, CVen, CTCOH, CBldTCA, zAUrntTCA, AUrnTCOGTCOH, TotCTCOH, CDCVG_Mole
   0.5    3.10   0.56   0.30    nan      nan    0.56   0.00886
   1.0    3.76   1.12   0.75    nan      nan    1.12   0.0349
   2.0    3.46   1.75   1.42    nan      nan    1.75   0.0461
   3.0    3.83   2.55   2.34    nan      nan    2.55   0.0337
   4.0    3.78   3.48   3.01    nan      nan    3.48   0.0313
   4.25   2.90   3.73   2.58    0.98    28.92   3.73   0.0241
   4.5    2.11   3.52   3.10    nan      nan    3.52   0.0132
   5.0    1.09   3.78   3.26    1.21    31.85   3.78   0.00552
   6.0    nan    3.79   4.21    1.42    40.01   3.79   0.00417
   8.0    nan    3.30   4.99    2.05    56.31   3.30   0.000671
  10.0    nan    2.96   5.46    3.12    68.48   2.96   nan
  12.0    nan    2.71   5.74    3.60    78.80   2.71   nan
  14.0    nan    2.38   6.69    4.09    89.82   2.38   nan
  16.0    nan    2.04   6.85    4.57    98.66   2.04   nan
  18.0    nan    1.89   7.14    4.86   105.25   1.89   nan
  20.0    nan    1.57   9.85    5.28   112.29   1.57   nan
  22.0    nan    1.40   9.32    5.98   122.73   1.40   nan
  25.5    nan    nan    nan     8.14   141.62   nan    nan
  36.5    nan    nan    nan     8.94   150.29   nan    nan
  44.0    nan    nan    nan    10.97   162.32   nan    nan
  47.0    nan    nan    nan    11.58   165.74   nan    nan
  50.5    nan    nan    8.87    nan      nan    nan    nan
  54.0    nan    nan    nan    13.48   173.84   nan    nan
  61.5    nan    nan    nan    15.33   178.30   nan    nan
  69.25   nan    nan    nan    17.47   182.24   nan    nan
  74.0    nan    nan    8.08    nan      nan    nan    nan
  85.0    nan    nan    nan    21.65   185.01   nan    nan
  93.5    nan    nan    nan    21.65   186.89   nan    nan
  98.5    nan    nan    3.82    nan      nan    nan    nan
```

```
TCE Inhalation 53.1 ppm for 4 hours -- Male subject 4
Hours, CVen, CTCOH, CBldTCA, zAUrntTCA, AUrnTCOGTCOH, TotCTCOH
    0.5    0.67   0.0    0.0     nan     nan    nan
    1.0    1.37   0.43   0.29    nan     nan    0.43
    2.0    1.96   1.20   0.77    nan     nan    1.20
    3.0    1.92   1.26   1.33    nan     nan    1.26
    4.0    2.08   1.69   1.84    nan     nan    1.69
    4.25   1.13   1.66   1.93    nan     nan    1.66
    4.5    0.76   1.60   2.07    nan     nan    1.60
    5.0    0.42   1.58   2.27    nan     nan    1.58
    5.25   nan    nan    nan     1.00    5.26   1.51
    6.0    0.30   1.51   2.94    1.53    8.23   1.44
    8.0    0.21   1.44   3.58    3.34   13.05   1.52
   10.0    0.15   1.52   3.72    6.01   16.30   1.14
   12.0    nan    1.14   3.98    7.60   19.05   1.05
   14.0    nan    1.05   4.40   13.02   24.62   1.04
   16.0    nan    1.04   4.58   14.83   26.97   1.06
   18.0    nan    1.06   4.86   16.67   29.06   0.45
   20.0    nan    0.45   5.73   18.69   30.62   0.75
```

22.0	nan	0.75	4.22	21.30	32.53	nan
25.0	nan	nan	nan	21.95	33.35	nan
30.0	nan	nan	nan	26.24	35.43	nan
38.0	nan	nan	nan	31.79	37.99	nan
44.75	nan	nan	5.00	40.44	38.21	nan
45.75	nan	nan	nan	40.86	39.06	nan
49.75	nan	nan	nan	42.64	39.63	nan
53.25	nan	nan	nan	42.94	39.70	nan
61.25	nan	nan	nan	43.80	39.90	nan
62.75	nan	nan	nan	44.54	40.23	nan
68.75	nan	nan	4.72	nan	nan	nan
79.0	nan	nan	nan	48.73	40.67	nan
100.5	nan	nan	4.47	nan	nan	nan

TCE Inhalation 97.8 ppm for 4 hours -- Male subject 4

Hours,	CVen,	CTCOH,	CBldTCA,	CAlvPPM,	zAUrntTCA,	AUrnTCOGTCOH,	TotCTCOH,	CDCVG_Mole
0.5	0.64	nan	0.21	nan	nan	nan	nan	0.00886
1.0	0.94	0.47	0.49	nan	nan	nan	0.47	0.0349
2.0	1.35	1.10	1.10	nan	nan	nan	1.10	0.0461
3.0	1.62	1.58	1.67	nan	nan	nan	1.58	0.0337
4.0	1.56	2.10	2.52	24.679	nan	nan	2.10	0.0313
4.25	1.16	2.21	2.44	6.422	nan	nan	2.21	0.0241
4.5	0.77	2.20	2.71	4.394	0.32	11.60	2.20	0.0132
5.0	0.37	2.15	3.18	2.691	0.41	13.64	2.15	0.00552
6.0	0.23	1.94	3.46	1.388	1.04	18.54	1.94	0.00417
8.0	0.19	1.88	4.26	1.198	1.32	25.00	1.88	0.000671
10.0	0.17	1.61	4.93	0.592	2.51	33.99	1.61	nan
12.0	nan	1.39	5.43	0.470	4.77	42.10	1.39	nan
14.0	nan	1.26	5.85	0.369	7.29	50.19	1.26	nan
16.0	nan	1.06	6.02	0.351	10.23	60.58	1.06	nan
18.0	nan	0.95	6.18	nan	11.50	64.73	0.95	nan
20.0	nan	0.88	6.35	nan	13.03	70.85	0.88	nan
22.0	nan	0.77	6.52	nan	14.26	77.69	0.77	nan
30.5	nan	nan	nan	nan	17.65	79.75	nan	nan
35.75	nan	nan	nan	nan	18.58	80.14	nan	nan
48.0	nan	nan	12.88	nan	nan	nan	nan	nan
51.75	nan	nan	nan	nan	18.58	80.23	nan	nan
56.75	nan	nan	nan	nan	18.58	80.32	nan	nan
61.5	nan	nan	nan	nan	18.95	80.66	nan	nan
70.0	nan	nan	nan	nan	20.95	81.44	nan	nan
71.75	nan	nan	6.25	nan	nan	nan	nan	nan
72.75	nan	nan	nan	nan	22.77	82.38	nan	nan
77.0	nan	nan	nan	nan	25.76	82.74	nan	nan
82.75	nan	nan	nan	nan	30.01	83.28	nan	nan
85.75	nan	nan	nan	nan	30.70	83.35	nan	nan
93.75	nan	nan	nan	nan	34.88	83.79	nan	nan
101.0	nan	nan	5.07	nan	nan	nan	nan	nan

TCE Inhalation 105.5 ppm for 4 hours -- Male subject 5

Hours,	CVen,	CTCOH,	CBldTCA,	zAUrntTCA,	AUrnTCOGTCOH,	TotCTCOH,	CDCVG_Mole
0.5	1.69	nan	0.24	nan	nan	nan	0.00886
1.0	2.50	0.37	0.60	nan	nan	0.37	0.0349
2.0	3.50	1.41	1.24	nan	nan	1.41	0.0461
3.0	4.24	2.40	2.71	nan	nan	2.40	0.0337
4.0	4.75	3.59	nan	nan	nan	3.59	0.0313
4.25	3.76	4.16	4.23	1.74	0.0	4.16	0.0241
4.5	2.20	3.73	3.86	nan	nan	3.73	0.0132
5.0	0.96	3.65	3.92	nan	nan	3.65	0.00552
6.0	nan	nan	nan	2.77	8.69	nan	0.00417
6.5	0.53	3.63	4.54	nan	nan	3.63	nan
8.0	0.26	2.60	5.71	3.94	18.39	2.60	0.000671
10.0	0.17	2.82	6.21	5.52	27.48	2.82	nan
12.0	0.17	1.84	nan	7.66	37.49	1.84	nan
14.0	nan	1.55	7.96	9.62	44.58	1.55	nan
16.0	nan	1.59	9.08	11.69	51.78	1.59	nan
18.0	nan	1.06	8.30	13.57	56.11	1.06	nan
20.0	nan	1.23	8.43	20.39	60.47	1.23	nan
22.0	nan	0.75	8.95	26.25	64.77	0.75	nan

24.5	nan	nan	nan	30.32	66.98	nan	nan
31.0	nan	nan	nan	40.91	75.49	nan	nan
35.5	nan	nan	nan	50.70	79.43	nan	nan
45.0	nan	nan	nan	65.02	82.13	nan	nan
49.75	nan	nan	nan	65.02	85.29	nan	nan
53.75	nan	nan	nan	78.15	88.15	nan	nan
54.75	nan	nan	nan	79.79	88.66	nan	nan
59.5	nan	nan	nan	83.82	89.44	nan	nan
69.0	nan	nan	nan	93.09	90.60	nan	nan
69.75	nan	nan	5.51	nan	nan	nan	nan
70.75	nan	nan	nan	98.82	91.71	nan	nan
72.0	nan	nan	nan	100.66	91.84	nan	nan
74.5	nan	nan	nan	112.13	92.37	nan	nan
77.0	nan	nan	nan	117.83	93.07	nan	nan
84.0	nan	nan	nan	118.82	93.79	nan	nan
86.0	nan	nan	nan	119.30	94.17	nan	nan
92.75	nan	nan	nan	120.02	94.55	nan	nan
93.5	nan	nan	3.55	nan	nan	nan	nan

TCE Inhalation 102.6 ppm for 4 hours -- Male subject 6

Hours	CVen	CTCOH	CBldTCA	zAUrntTCA	AUrnTCOGTCOH	TotCTCOH	CDCVG_Mole
0.5	1.93	0.45	0.23	nan	nan	0.45	0.00886
1.0	2.34	0.77	0.49	nan	nan	0.77	0.0349
2.0	2.84	1.51	1.07	nan	nan	1.51	0.0461
3.0	3.40	2.41	1.89	0.488	32.70	2.41	0.0337
4.0	3.41	3.30	2.87	nan	nan	3.30	0.0313
4.25	2.20	3.64	3.69	nan	nan	3.64	0.0241
4.5	1.66	3.67	3.87	nan	nan	3.67	0.0132
4.75	nan	nan	nan	0.961	60.26	nan	nan
5.0	0.89	3.48	3.59	nan	nan	3.48	0.00552
6.0	0.38	3.05	4.18	nan	nan	3.05	0.00417
6.5	nan	nan	nan	2.09	97.98	nan	nan
8.0	nan	2.52	4.71	nan	nan	2.52	0.000671
8.25	nan	nan	nan	2.96	130.67	nan	nan
10.0	nan	2.38	5.46	5.56	182.90	2.38	nan
12.0	nan	2.16	5.67	7.17	204.64	2.16	nan
14.0	nan	1.73	5.97	8.37	224.53	1.73	nan
15.5	nan	nan	nan	9.09	233.79	nan	nan
16.0	nan	1.48	6.05	nan	nan	1.48	nan
17.5	nan	nan	nan	9.70	240.99	nan	nan
18.0	nan	1.12	6.22	10.13	245.36	1.12	nan
19.5	nan	nan	nan	10.99	253.46	nan	nan
20.0	nan	1.01	7.54	11.24	255.90	1.01	nan
21.3	nan	nan	nan	11.88	261.17	nan	nan
22.0	nan	0.85	7.26	12.36	265.40	0.85	nan
23.0	nan	nan	nan	13.03	269.76	nan	nan
35.5	nan	nan	nan	14.18	271.64	nan	nan
40.75	nan	nan	nan	16.14	276.15	nan	nan
46.75	nan	nan	8.43	18.07	277.54	nan	nan
47.0	nan	nan	nan	19.06	277.83	nan	nan
52.25	nan	nan	nan	20.35	278.12	nan	nan
55.25	nan	nan	nan	23.68	278.81	nan	nan
68.0	nan	nan	nan	24.71	278.88	nan	nan
69.75	nan	nan	nan	27.02	279.07	nan	nan
71.5	nan	nan	3.86	nan	nan	nan	nan
95.5	nan	nan	3.55	nan	nan	nan	nan

TCE Inhalation 102.0 ppm for 4 hours -- Male subject 7

Hours	CVen	CTCOH	CBldTCA	CAlvPPM	zAUrntTCA	AUrnTCOGTCOH	TotCTCOH	CDCVG_Mole
0.5	0.76	0.0	0.11	nan	nan	nan	nan	0.00886
1.0	0.86	0.52	0.36	nan	nan	nan	0.52	0.0349
2.0	1.15	1.35	1.07	nan	nan	nan	1.35	0.0461
3.0	1.15	1.87	1.55	nan	nan	nan	1.87	0.0337
4.0	1.23	2.50	2.31	12.386	nan	nan	2.50	0.0313
4.25	0.77	2.59	2.03	3.305	nan	nan	2.59	0.0241
4.5	0.46	2.58	2.16	2.478	1.36	16.05	2.58	0.0132
5.0	0.34	2.25	2.35	1.567	1.66	18.22	2.25	0.00552
6.0	0.21	2.15	2.53	0.577	2.70	25.28	2.15	0.00417

8.0	0.15	1.98	3.61	0.317	4.22	34.46	1.98	0.000671
10.0	nan	1.56	3.93	0.286	6.04	43.49	1.56	nan
12.0	nan	1.02	4.57	nan	8.04	49.91	1.02	nan
14.0	nan	1.26	4.50	nan	10.37	55.78	1.26	nan
16.0	nan	0.89	5.02	nan	13.33	59.33	0.89	nan
18.0	nan	0.79	5.10	nan	16.55	65.07	0.79	nan
20.0	nan	0.73	5.07	nan	20.04	68.36	0.73	nan
22.0	nan	0.70	5.91	nan	23.89	71.48	0.70	nan
25.25	nan	nan	nan	nan	30.02	76.10	nan	nan
32.0	nan	nan	nan	nan	35.07	81.25	nan	nan
35.25	nan	nan	nan	nan	38.42	83.82	nan	nan
43.5	nan	nan	nan	nan	43.06	86.11	nan	nan
51.0	nan	nan	6.38	nan	46.65	87.66	nan	nan
53.25	nan	nan	nan	nan	48.88	88.38	nan	nan
57.0	nan	nan	nan	nan	54.83	89.39	nan	nan
58.25	nan	nan	nan	nan	57.31	89.71	nan	nan
59.75	nan	nan	nan	nan	59.49	89.92	nan	nan
63.75	nan	nan	nan	nan	62.36	89.92	nan	nan
67.5	nan	nan	nan	nan	66.44	90.38	nan	nan
73.0	nan	nan	nan	nan	70.15	91.07	nan	nan
78.0	nan	nan	5.33	nan	73.57	91.55	nan	nan
80.5	nan	nan	nan	nan	75.42	91.79	nan	nan
82.75	nan	nan	nan	nan	77.73	91.94	nan	nan
84.25	nan	nan	nan	nan	78.87	92.03	nan	nan
85.0	nan	nan	nan	nan	80.37	92.22	nan	nan
87.5	nan	nan	nan	nan	83.60	92.37	nan	nan
92.0	nan	nan	nan	nan	86.81	92.55	nan	nan
101.0	nan	nan	4.01	nan	nan	nan	nan	nan

TCE Inhalation 101.1 ppm for 4 hours -- Male subject 8

Hours	CVen	CTCOH	CBldTCA	CAlvPPM	zAUrntTCA	AUrnTCOGTCOH	TotCTCOH	CDCVG_Mole
0.5	0.59	0.28	0.36	nan	nan	nan	0.28	0.00886
1.0	0.85	0.76	0.84	nan	nan	nan	0.76	0.0349
2.0	1.1	1.92	1.73	nan	nan	nan	1.92	0.0461
3.0	1.04	1.69	2.60	nan	nan	nan	1.69	0.0337
4.0	1.18	2.34	3.42	21.575	nan	nan	2.34	0.0313
4.0	nan	nan	nan	14.272	nan	nan	nan	nan
4.0	nan	nan	nan	10.77	nan	nan	nan	nan
4.0	nan	nan	nan	7.056	nan	nan	nan	nan
4.25	nan	nan	nan	5.876	nan	nan	2.34	0.0241
4.25	0.64	2.34	3.90	5.773	nan	nan	nan	nan
4.5	0.42	2.16	3.67	5.010	nan	nan	2.16	0.0132
4.75	nan	nan	nan	nan	0.93	40.71	nan	nan
5.0	0.19	2.13	4.47	2.498	nan	nan	2.13	0.00552
6.0	nan	1.95	5.00	1.713	nan	nan	1.95	0.00417
8.0	nan	1.61	5.95	1.263	3.02	69.81	1.61	0.000671
10.0	nan	1.33	6.74	1.029	nan	nan	1.33	nan
12.0	nan	1.58	7.12	0.936	nan	nan	1.58	nan
14.0	nan	0.84	7.75	0.809	5.95	89.76	0.84	nan
16.0	nan	0.77	8.22	0.738	7.07	96.80	0.77	nan
18.0	nan	0.57	8.17	0.683	8.28	102.69	0.57	nan
20.0	nan	0.76	9.01	nan	nan	nan	0.76	nan
20.25	nan	nan	nan	nan	9.63	107.93	nan	nan
24.75	nan	nan	nan	nan	13.46	121.30	nan	nan
29.0	nan	nan	nan	nan	15.73	128.51	nan	nan
32.75	nan	nan	nan	nan	20.11	135.51	nan	nan
35.25	nan	nan	nan	nan	22.71	138.05	nan	nan
39.0	nan	nan	nan	nan	24.07	140.20	nan	nan
44.25	nan	nan	nan	nan	25.60	142.48	nan	nan
49.75	nan	nan	10.66	nan	27.51	144.47	nan	nan
56.0	nan	nan	nan	nan	29.60	144.96	nan	nan
58.75	nan	nan	nan	nan	33.36	145.55	nan	nan
68.25	nan	nan	nan	nan	39.61	146.67	nan	nan
74.0	nan	nan	8.60	nan	43.70	147.09	nan	nan
76.0	nan	nan	nan	nan	45.78	147.25	nan	nan
78.0	nan	nan	nan	nan	48.52	147.38	nan	nan
81.0	nan	nan	nan	nan	51.21	147.50	nan	nan
82.5	nan	nan	nan	nan	53.54	147.62	nan	nan
92.0	nan	nan	nan	nan	60.72	147.98	nan	nan

95.25	nan	nan	7.46	nan	nan	nan	nan	nan
264.0	nan	nan	3.13	nan	nan	nan	nan	nan

TCE Inhalation 103.4 ppm for 4 hours -- Male subject 9

Hours	CVen	CTCOH	CBldTCA	zAUrntTCA	AUrnTCOGTCOH	TotCTCOH	CDCVG_Mole
0.5	2.69	0.47	0.43	nan	nan	0.47	0.00886
1.0	2.98	0.68	1.00	nan	nan	0.68	0.0349
2.0	3.51	1.51	2.15	nan	nan	1.51	0.0461
3.0	3.58	3.58	3.40	nan	nan	3.58	0.0337
4.0	2.88	2.72	4.94	nan	nan	2.72	0.0313
4.25	1.96	2.87	5.42	nan	nan	2.87	0.0241
4.5	1.53	2.77	5.67	0.935	40.02	2.77	0.0132
5.0	nan	nan	nan	nan	nan	nan	0.00552
5.75	0.81	2.63	5.83	1.34	40.67	2.63	nan
6.0	0.52	2.30	5.99	4.10	57.48	2.30	0.00417
8.0	0.32	1.90	7.23	6.10	76.60	1.90	0.000671
10.0	0.27	1.59	7.96	9.74	99.19	1.59	nan
12.0	0.24	1.28	8.14	13.29	115.98	1.28	nan
14.0	0.22	1.23	8.39	16.29	126.00	1.23	nan
16.0	0.22	1.06	8.36	20.29	136.55	1.06	nan
18.0	0.20	0.98	8.83	22.87	143.51	0.98	nan
20.0	0.16	0.72	8.96	24.83	150.54	0.72	nan
22.0	0.16	0.71	9.51	29.98	163.57	0.71	nan
45.0	nan	nan	10.75	nan	nan	nan	nan
45.5	nan	nan	nan	56.81	196.37	nan	nan
47.5	nan	nan	nan	61.82	197.62	nan	nan
49.0	nan	nan	nan	64.84	198.48	nan	nan
50.5	nan	nan	nan	67.02	199.33	nan	nan
54.0	nan	nan	nan	74.27	201.12	nan	nan
57.25	nan	nan	nan	76.87	201.12	nan	nan
59.0	nan	nan	nan	78.68	201.73	nan	nan
61.0	nan	nan	nan	61.05	202.15	nan	nan
64.0	nan	nan	nan	88.53	202.88	nan	nan
68.0	nan	nan	nan	90.31	203.60	nan	nan
69.0	nan	nan	9.21	nan	nan	nan	nan
74.5	nan	nan	nan	92.43	204.11	nan	nan
80.25	nan	nan	nan	95.17	204.47	nan	nan
82.5	nan	nan	nan	97.12	204.92	nan	nan
84.25	nan	nan	nan	100.02	205.07	nan	nan
85.5	nan	nan	nan	100.76	205.15	nan	nan
87.0	nan	nan	nan	103.23	205.30	nan	nan
93.0	nan	nan	7.94	nan	nan	nan	nan
264.0	nan	nan	1.94	nan	nan	nan	nan

TCE Inhalation 55.1 ppm for 4 hours -- Female subject 1

Hours	CVen	CTCOH	CBldTCA	zAUrntTCA	AUrnTCOGTCOH	TotCTCOH
0.5	1.00	0.32	0.16	nan	nan	0.32
1.0	1.29	0.49	0.46	nan	nan	0.49
2.0	1.38	0.85	1.15	nan	nan	0.85
3.0	1.70	0.97	1.53	nan	nan	0.97
4.0	1.72	1.20	1.90	nan	nan	1.20
4.25	1.08	1.14	2.10	nan	nan	1.14
4.5	1.17	1.18	2.18	0.64	20.08	1.18
5.0	0.55	1.13	2.13	0.76	22.91	1.13
6.0	0.39	nan	2.56	0.85	24.87	nan
8.0	0.22	nan	3.32	1.83	28.94	nan
10.0	nan	0.70	2.83	2.57	36.46	0.70
12.0	nan	0.60	2.98	3.36	39.14	0.60
14.0	nan	0.52	3.42	3.94	42.64	0.52
16.0	nan	0.55	3.44	5.12	45.16	0.55
18.0	nan	0.54	3.31	6.03	53.64	0.54
20.0	nan	0.45	4.15	6.67	56.34	0.45
22.0	nan	0.35	4.07	7.30	57.08	0.35
23.25	nan	nan	nan	7.60	57.64	nan
25.25	nan	nan	nan	7.96	58.45	nan
27.5	nan	nan	nan	8.60	60.33	nan
29.5	nan	nan	nan	8.89	61.44	nan
31.0	nan	nan	nan	9.21	62.83	nan
33.0	nan	nan	nan	9.86	67.36	nan

35.0	nan	nan	nan	9.66	68.30	nan
40.0	nan	nan	nan	11.19	69.92	nan
42.0	nan	nan	nan	11.85	70.88	nan
43.0	nan	nan	nan	12.35	71.09	nan
44.5	nan	nan	3.70	12.73	71.59	nan
46.5	nan	nan	nan	13.49	71.99	nan
50.0	nan	nan	nan	14.31	72.60	nan
52.0	nan	nan	nan	15.73	73.60	nan
53.5	nan	nan	nan	16.12	73.93	nan
54.5	nan	nan	nan	16.34	74.27	nan
57.0	nan	nan	nan	16.93	74.26	nan
58.5	nan	nan	nan	17.24	74.56	nan
59.25	nan	nan	nan	17.85	74.71	nan
64.0	nan	nan	nan	18.13	74.77	nan
68.25	nan	nan	3.31	18.53	75.16	nan
70.75	nan	nan	nan	19.18	75.34	nan
72.75	nan	nan	nan	19.42	75.52	nan
74.75	nan	nan	nan	20.00	75.75	nan
77.0	nan	nan	nan	20.58	75.81	nan
80.25	nan	nan	nan	20.79	76.05	nan
81.5	nan	nan	nan	20.93	76.06	nan
82.5	nan	nan	nan	21.82	76.12	nan
83.5	nan	nan	nan	21.37	76.15	nan
90.25	nan	nan	nan	21.56	76.30	nan
91.5	nan	nan	nan	21.69	76.34	nan
92.25	nan	nan	nan	21.87	76.39	nan
93.25	nan	nan	1.02	nan	nan	nan

TCE Inhalation 101.4 ppm for 4 hours -- Female subject 1

Hours	CVen	CTCOH	CBldTCA	zAUrntTCA	AUrnTCOGTCOH	TotCTCOH	CDCVG_Mole
0.5	1.18	nan	nan	nan	nan	nan	0.0032
1.0	2.17	0.74	nan	nan	nan	0.74	0.00868
2.0	2.30	1.38	0.91	nan	nan	1.38	0.0106
3.0	2.41	1.93	1.75	nan	nan	1.93	0.0127
4.0	2.65	2.41	2.65	nan	nan	2.41	0.0133
4.25	1.84	2.40	2.54	0.31	35.78	2.4	0.0087
4.5	1.17	2.33	2.65	nan	nan	2.33	0.00508
5.0	0.62	2.17	2.73	0.39	44.4	2.17	0.00229
6.0	0.38	1.94	3.26	0.64	54.4	1.94	0.00074
8.0	nan	1.81	3.58	1.21	72.58	1.81	nan
10.0	nan	1.38	4.50	1.66	90.61	1.38	nan
12.0	nan	1.17	4.02	2.16	104.44	1.17	nan
14.0	nan	1.25	4.17	2.96	116.90	1.25	nan
16.0	nan	1.01	4.45	3.66	127.49	1.01	nan
18.0	nan	0.88	4.90	4.37	127.49	0.88	nan
20.0	nan	0.74	5.26	5.44	136.49	0.74	nan
22.0	nan	0.70	5.94	6.66	144.45	0.7	nan
24.25	nan	nan	nan	7.63	147.89	nan	nan
27.0	nan	nan	nan	8.16	150.61	nan	nan
28.25	nan	nan	nan	8.71	154.52	nan	nan
30.0	nan	nan	nan	10.30	157.72	nan	nan
32.5	nan	nan	nan	10.92	160.74	nan	nan
34.25	nan	nan	nan	11.77	163.47	nan	nan
36.0	nan	nan	nan	12.45	165.86	nan	nan
43.25	nan	nan	nan	13.71	167.54	nan	nan
45.5	nan	nan	nan	14.04	168.21	nan	nan
46.5	nan	nan	6.68	nan	nan	nan	nan
48.0	nan	nan	nan	15.07	169.24	nan	nan
51.5	nan	nan	nan	15.98	170.26	nan	nan
54.0	nan	nan	nan	16.51	171.66	nan	nan
56.5	nan	nan	nan	17.00	172.85	nan	nan
58.25	nan	nan	nan	17.60	173.70	nan	nan
59.5	nan	nan	nan	19.57	175.02	nan	nan
67.5	nan	nan	nan	19.76	175.31	nan	nan
70.25	nan	nan	5.20	20.25	175.67	nan	nan
72.25	nan	nan	nan	21.31	176.21	nan	nan
75.0	nan	nan	nan	22.08	176.60	nan	nan
77.5	nan	nan	nan	22.65	177.07	nan	nan
81.5	nan	nan	nan	24.79	178.04	nan	nan
84.0	nan	nan	nan	30.86	178.43	nan	nan

89.0	nan	nan	nan	31.05	178.65	nan	nan
91.25	nan	nan	nan	31.06	178.94	nan	nan
93.75	nan	nan	3.60	nan	nan	nan	nan

TCE Inhalation 53.0 ppm for 4 hours -- Female subject 2

Hours	CVen	CTCOH	CBldTCA	zAUrntTCA	AUrnTCOGTCOH	TotCTCOH
0.5	0.93	nan	nan	nan	nan	nan
1.0	1.33	0.33	0.38	nan	nan	0.33
2.0	1.65	0.63	1.23	nan	nan	0.63
3.0	1.85	0.79	1.96	nan	nan	0.79
4.0	1.45	0.98	2.80	nan	nan	0.98
4.25	0.94	0.83	2.81	nan	nan	0.83
4.5	0.63	0.83	3.23	nan	nan	0.83
5.0	0.32	0.90	3.34	1.35	4.42	0.90
6.0	0.18	0.89	3.72	4.49	6.71	0.89
8.0	nan	0.76	4.88	7.17	12.00	0.76
10.0	nan	0.66	4.93	9.38	15.40	0.66
12.0	nan	0.67	5.28	10.36	16.73	0.67
14.0	nan	0.54	5.18	11.91	20.35	0.54
16.0	nan	0.48	5.37	13.46	23.49	0.48
18.0	nan	0.47	6.03	14.70	25.44	0.47
20.0	nan	nan	4.87	15.64	25.44	nan
22.0	nan	0.35	6.66	16.49	26.96	0.35
25.0	nan	nan	nan	22.11	30.55	nan
30.0	nan	nan	nan	23.27	32.71	nan
38.0	nan	nan	nan	26.03	34.38	nan
45.0	nan	nan	6.66	27.35	34.88	nan
49.75	nan	nan	nan	33.94	37.25	nan
53.25	nan	nan	nan	35.83	38.53	nan
61.25	nan	nan	nan	42.58	41.16	nan
63.0	nan	nan	nan	43.36	41.38	nan
68.0	nan	nan	nan	50.68	43.01	nan
69.0	nan	nan	5.27	nan	nan	nan
75.75	nan	nan	nan	52.36	43.29	nan
79.75	nan	nan	nan	53.79	43.53	nan
96.75	nan	nan	nan	54.16	43.66	nan
97.0	nan	nan	nan	55.93	43.85	nan
100.5	nan	nan	2.27	nan	nan	nan

TCE Inhalation 97.7 ppm for 4 hours -- Female subject 2

Hours	CVen	CTCOH	CBldTCA	CAlvPPM	zAUrntTCA	AUrnTCOGTCOH	TotCTCOH	CDCVG_Mole
0.5	0.83	nan	0.44	nan	nan	nan	nan	0.0032
1.0	0.99	nan	0.97	nan	nan	nan	nan	0.00868
2.0	1.20	0.53	2.16	nan	nan	nan	0.53	0.0106
3.0	1.59	0.83	3.79	nan	nan	nan	0.83	0.0127
4.0	2.03	1.27	5.12	22.398	nan	nan	1.27	0.0133
4.25	1.33	0.92	5.35	7.317	nan	nan	0.92	0.0087
4.5	0.87	0.85	5.60	5.917	0.30	11.67	0.85	0.00508
5.0	0.42	1.17	5.88	2.903	0.56	14.56	1.17	0.00229
6.0	0.21	1.03	6.55	1.382	1.75	20.78	1.03	0.00074
8.0	0.22	0.86	7.30	0.982	1.97	25.55	0.86	nan
10.0	0.15	0.80	7.66	0.691	3.75	34.83	0.80	nan
12.0	nan	0.71	8.61	0.524	6.58	45.33	0.71	nan
14.0	nan	0.62	8.73	0.428	6.81	45.98	0.62	nan
16.0	nan	0.55	9.65	nan	8.64	54.21	0.55	nan
18.0	nan	0.48	8.29	nan	10.30	60.91	0.48	nan
20.0	nan	0.41	8.60	nan	12.13	68.01	0.41	nan
22.0	nan	nan	10.20	nan	13.64	73.35	nan	nan
32.0	nan	nan	nan	nan	15.77	75.14	nan	nan
34.25	nan	nan	nan	nan	18.03	79.52	nan	nan
37.0	nan	nan	nan	nan	18.16	79.97	nan	nan
48.0	nan	nan	6.15	nan	22.69	85.95	nan	nan
56.0	nan	nan	nan	nan	28.52	90.84	nan	nan
59.0	nan	nan	nan	nan	30.85	91.82	nan	nan
63.5	nan	nan	nan	nan	31.36	92.13	nan	nan
71.0	nan	nan	nan	nan	33.88	92.13	nan	nan
72.0	nan	nan	7.11	nan	nan	nan	nan	nan
76.0	nan	nan	nan	nan	37.20	95.09	nan	nan

85.5	nan	nan	nan	nan	41.32	96.05	nan	nan
87.25	nan	nan	nan	nan	42.86	96.34	nan	nan
88.0	nan	nan	nan	nan	49.42	96.45	nan	nan
94.75	nan	nan	nan	nan	54.14	97.45	nan	nan
101.25	nan	nan	6.73	nan	nan	nan	nan	nan

TCE Inhalation 102.5 ppm for 4 hours -- Female subject 3

Hours,	CVen,	CTCOH,	CBldTCA,	zAUrntTCA,	AUrnTCOGTCOH,	TotCTCOH,	CDCVG_Mole
0.5	1.11	0.22	0.21	nan	nan	0.22	0.0032
1.0	1.36	0.46	0.39	nan	nan	0.46	0.00868
2.0	2.11	1.18	1.05	nan	nan	1.18	0.0106
3.0	1.92	2.18	1.86	nan	nan	2.18	0.0127
4.0	2.30	3.03	3.46	nan	nan	3.03	0.0133
4.25	1.56	3.29	3.78	nan	nan	3.29	0.0087
4.5	1.26	3.67	3.91	0.51	44.83	3.67	0.00508
5.0	0.73	3.13	4.22	0.65	52.08	3.13	0.00229
6.0	0.42	2.57	4.67	nan	nan	2.57	0.00074
7.0	nan	nan	nan	1.26	77.84	nan	nan
8.0	nan	2.46	5.71	1.85	89.76	2.46	nan
10.0	nan	1.93	6.29	2.92	108.58	1.93	nan
12.0	nan	1.57	7.76	3.91	122.65	1.57	nan
14.0	nan	1.30	7.78	4.92	133.38	1.30	nan
16.0	nan	1.08	8.11	5.91	140.85	1.08	nan
18.0	nan	0.89	8.79	5.91	147.19	0.89	nan
20.0	nan	0.56	9.05	7.12	151.76	0.56	nan
22.0	nan	0.65	9.34	9.55	155.86	0.65	nan
30.75	nan	nan	nan	15.22	169.38	nan	nan
33.75	nan	nan	nan	17.85	174.67	nan	nan
35.5	nan	nan	nan	19.66	175.78	nan	nan
40.75	nan	nan	nan	24.08	179.31	nan	nan
46.25	nan	0.30	9.58	26.68	179.77	0.30	nan
47.0	nan	nan	nan	27.91	179.97	nan	nan
52.25	nan	nan	nan	30.49	180.44	nan	nan
55.25	nan	nan	nan	35.74	181.52	nan	nan
68.0	nan	nan	nan	35.75	184.09	nan	nan
69.75	nan	nan	nan	36.78	184.16	nan	nan
70.0	nan	nan	7.93	nan	nan	nan	nan
74.0	nan	nan	nan	37.71	184.26	nan	nan
76.0	nan	nan	nan	41.25	184.70	nan	nan
78.0	nan	nan	nan	45.21	185.20	nan	nan
80.25	nan	nan	nan	46.43	185.35	nan	nan
81.5	nan	nan	nan	47.22	185.42	nan	nan
82.25	nan	nan	nan	47.91	185.51	nan	nan
92.5	nan	nan	nan	49.66	185.81	nan	nan
93.75	nan	nan	nan	50.98	185.91	nan	nan
94.75	nan	nan	6.69	51.67	185.95	nan	nan

TCE Inhalation 102.0 ppm for 4 hours -- Female subject 4

Hours,	CVen,	CTCOH,	CBldTCA,	zAUrntTCA,	AUrnTCOGTCOH,	TotCTCOH,	CDCVG_Mole
0.5	0.81	0.33	0.40	nan	nan	0.33	0.0032
1.0	0.88	0.57	0.97	nan	nan	0.57	0.00868
2.0	1.09	1.01	1.72	nan	nan	1.01	0.0106
3.0	1.03	1.25	2.64	nan	nan	1.25	0.0127
4.0	1.13	1.79	3.41	nan	nan	1.79	0.0133
4.25	0.59	1.64	3.62	nan	nan	1.64	0.0087
4.5	0.47	1.54	3.86	0.44	12.63	1.54	0.00508
5.0	0.30	1.43	4.39	nan	nan	1.43	0.00229
6.0	0.18	1.27	4.80	0.71	17.83	1.27	0.00074
8.0	0.15	0.95	5.73	1.31	26.05	0.95	nan
10.0	nan	1.01	6.79	2.28	30.40	1.01	nan
12.0	nan	0.90	7.55	3.48	36.72	0.90	nan
14.0	nan	0.88	7.68	4.64	41.26	0.88	nan
16.0	nan	0.74	7.98	5.64	44.27	0.74	nan
18.0	nan	0.69	9.27	6.76	47.94	0.69	nan
20.0	nan	0.63	8.91	7.66	50.31	0.63	nan
22.0	nan	0.61	9.12	8.89	53.17	0.61	nan
26.0	nan	nan	nan	10.64	57.90	nan	nan
33.25	nan	nan	nan	13.81	65.27	nan	nan
38.0	nan	nan	nan	14.11	65.80	nan	nan

45.0	nan	nan	nan	15.44	69.74	nan	nan
46.0	nan	nan	11.31	nan	nan	nan	nan
49.0	nan	nan	nan	16.00	69.74	nan	nan
55.0	nan	nan	nan	23.20	72.07	nan	nan
58.5	nan	nan	nan	22.40	73.58	nan	nan
61.5	nan	nan	nan	24.10	75.39	nan	nan
66.5	nan	nan	nan	29.10	76.98	nan	nan
70.75	nan	nan	nan	32.60	79.89	nan	nan
74.75	nan	nan	nan	36.20	80.98	nan	nan
75.75	nan	nan	10.49	nan	nan	nan	nan
80.5	nan	nan	nan	36.80	82.20	nan	nan
82.5	nan	nan	nan	37.50	82.57	nan	nan
85.0	nan	nan	nan	37.79	82.74	nan	nan
93.5	nan	nan	nan	45.72	83.41	nan	nan
94.25	nan	nan	8.47	nan	nan	nan	nan

TCE Inhalation 102.0 ppm for 4 hours -- Female subject 5

Hours,	CVen,	CTCOH,	CBldTCA,	CAlvPPM,	zAUrntTCA,	AUrnTCOGTCOH,	TotCTCOH,	CDCVG_Mole
0.5	0.74	nan	0.25	nan	nan	nan	nan	0.0032
1.0	1.00	0.41	0.76	nan	nan	nan	0.41	0.00868
2.0	1.27	0.78	1.48	nan	nan	nan	0.78	0.0106
3.0	1.45	1.04	2.21	nan	nan	nan	1.04	0.0127
4.0	1.19	1.18	2.79	nan	nan	nan	1.18	0.0133
4.25	0.81	1.17	2.78	4.243	nan	nan	1.17	0.0087
4.5	0.66	1.18	3.12	2.798	0.69	9.98	1.18	0.00508
5.0	0.46	1.18	3.23	1.849	0.80	9.98	1.18	0.00229
6.0	0.25	nan	3.52	1.467	1.64	12.41	nan	0.00074
8.0	0.19	0.84	4.76	0.681	3.16	16.09	0.84	nan
10.0	nan	0.72	4.95	0.452	4.95	18.99	0.72	nan
12.0	nan	0.82	5.29	0.409	7.19	20.96	0.82	nan
14.0	nan	0.56	5.33	0.356	9.89	23.08	0.56	nan
16.0	nan	nan	nan	nan	13.14	24.46	nan	nan
18.0	nan	0.49	6.46	nan	17.46	26.22	0.49	nan
20.0	nan	0.41	6.91	nan	21.67	27.92	0.41	nan
22.0	nan	nan	7.10	nan	26.40	29.05	nan	nan
22.75	nan	nan	nan	nan	29.05	29.64	nan	nan
26.5	nan	nan	nan	nan	35.18	32.31	nan	nan
29.75	nan	nan	nan	nan	41.73	34.40	nan	nan
34.0	nan	nan	nan	nan	49.36	36.58	nan	nan
35.75	nan	nan	nan	nan	50.76	37.14	nan	nan
40.75	nan	nan	nan	nan	56.47	38.80	nan	nan
43.75	nan	nan	nan	nan	60.68	39.86	nan	nan
47.0	nan	nan	6.63	nan	69.00	40.61	nan	nan
49.75	nan	nan	nan	nan	73.32	41.58	nan	nan
53.5	nan	nan	nan	nan	76.81	42.31	nan	nan
56.0	nan	nan	nan	nan	79.16	42.94	nan	nan
58.0	nan	nan	nan	nan	81.70	43.30	nan	nan
59.75	nan	nan	nan	nan	83.84	43.53	nan	nan
60.0	nan	nan	nan	nan	84.56	43.60	nan	nan
61.75	nan	nan	nan	nan	86.11	43.78	nan	nan
67.75	nan	nan	nan	nan	91.59	44.79	nan	nan
70.5	nan	nan	5.28	nan	nan	nan	nan	nan
72.75	nan	nan	nan	nan	95.63	45.19	nan	nan
76.75	nan	nan	nan	nan	100.35	45.69	nan	nan
82.75	nan	nan	nan	nan	110.14	46.42	nan	nan
84.0	nan	nan	nan	nan	111.45	46.54	nan	nan
85.75	nan	nan	nan	nan	112.62	46.60	nan	nan
91.75	nan	nan	nan	nan	115.92	47.13	nan	nan

TCE Inhalation 101.0 ppm for 4 hours -- Female subject 6

Hours,	CVen,	CTCOH,	CBldTCA,	zAUrntTCA,	AUrnTCOGTCOH,	TotCTCOH,	CDCVG_Mole
0.52	0.53	0.35	0.39	nan	nan	0.35	0.0032
1.0	1.00	0.58	1.08	nan	nan	0.58	0.00868
2.0	0.97	0.86	1.90	0.0	0.0	0.86	0.0106
3.0	1.31	1.60	3.83	nan	nan	1.60	0.0127
4.0	1.48	2.03	4.48	nan	nan	2.03	0.0133
4.25	0.84	2.04	4.65	nan	nan	2.04	0.0087
4.5	0.58	1.93	4.80	2.51	37.76	1.93	0.00508

5.0	0.39	1.95	4.73	3.07	42.18	1.95	0.00229
6.0	nan	1.79	6.02	6.21	48.68	1.79	0.00074
8.0	nan	1.29	6.02	9.97	60.91	1.29	nan
10.0	nan	1.14	7.12	13.01	72.32	1.14	nan
12.0	nan	1.03	7.13	16.35	81.05	1.03	nan
14.0	nan	nan	nan	20.65	86.76	nan	nan
16.0	nan	nan	nan	23.23	94.78	nan	nan
18.0	nan	nan	nan	26.31	100.92	nan	nan
20.0	nan	nan	nan	26.31	105.91	nan	nan
25.25	nan	nan	nan	34.28	115.12	nan	nan
25.75	nan	nan	nan	34.84	116.22	nan	nan
30.0	nan	nan	nan	42.19	125.29	nan	nan
34.5	nan	nan	nan	51.62	131.36	nan	nan
38.0	nan	nan	nan	61.19	135.91	nan	nan
45.0	nan	nan	nan	75.52	143.62	nan	nan
46.75	nan	nan	9.10	nan	nan	nan	nan
49.25	nan	nan	nan	81.43	146.34	nan	nan
57.0	nan	nan	nan	92.21	149.70	nan	nan
60.5	nan	nan	nan	104.12	151.17	nan	nan
68.25	nan	nan	nan	116.32	153.38	nan	nan
72.5	nan	nan	nan	121.17	154.28	nan	nan
74.0	nan	nan	6.92	nan	nan	nan	nan
80.5	nan	nan	nan	131.94	155.70	nan	nan
84.25	nan	nan	nan	134.71	155.93	nan	nan
86.0	nan	nan	nan	136.09	156.09	nan	nan
93.5	nan	nan	nan	142.30	156.70	nan	nan
95.5	nan	nan	6.14	nan	nan	nan	nan

TCE Inhalation 103.3 ppm for 4 hours -- Female subject 7

Hours	CVen	CTCOH	CBldTCA	zAUrntTCA	AUrnTCOGTCOH	TotCTCOH	CDCVG_Mole
0.5	1.32	0.47	0.27	nan	nan	0.47	0.0032
1.0	1.68	0.68	0.70	nan	nan	0.68	0.00868
2.0	1.86	1.51	1.48	nan	nan	1.51	0.0106
3.0	2.37	2.15	2.80	nan	nan	2.15	0.0127
4.0	2.66	2.72	3.92	nan	nan	2.72	0.0133
4.25	2.10	2.87	3.86	nan	nan	2.87	0.0087
4.5	1.23	2.77	3.98	2.34	15.54	2.77	0.00508
5.0	0.83	2.63	4.55	2.92	18.22	2.63	0.00229
6.0	0.42	2.30	4.80	5.27	24.58	2.30	0.00074
8.0	0.33	1.90	5.96	8.33	33.76	1.90	nan
10.0	0.30	1.59	6.09	12.15	41.25	1.59	nan
12.0	nan	1.28	6.41	17.02	47.80	1.28	nan
14.0	nan	1.23	7.01	21.46	54.36	1.23	nan
16.0	nan	1.10	7.23	26.02	59.99	1.10	nan
18.0	nan	0.98	7.57	28.88	63.23	0.98	nan
20.0	nan	0.72	7.68	32.60	68.23	0.72	nan
22.0	nan	0.71	8.46	37.96	73.90	0.71	nan
43.3	nan	nan	nan	80.45	110.18	nan	nan
45.0	nan	nan	8.75	85.25	112.61	nan	nan
47.5	nan	nan	nan	87.93	113.70	nan	nan
49.0	nan	nan	nan	91.55	115.14	nan	nan
53.5	nan	nan	nan	99.63	118.20	nan	nan
61.25	nan	nan	nan	110.21	122.07	nan	nan
67.25	nan	nan	nan	114.43	124.30	nan	nan
69.0	nan	nan	7.73	nan	nan	nan	nan
70.5	nan	nan	nan	118.52	125.29	nan	nan
74.5	nan	nan	nan	123.23	126.29	nan	nan
77.25	nan	nan	nan	128.78	127.48	nan	nan
83.25	nan	nan	nan	133.51	128.07	nan	nan
84.25	nan	nan	nan	134.95	128.31	nan	nan
85.0	nan	nan	nan	136.29	128.49	nan	nan
90.5	nan	nan	nan	143.83	129.56	nan	nan
93.0	nan	nan	5.72	nan	nan	nan	nan
264.0	nan	nan	0.53	nan	nan	nan	nan

TCE Inhalation 102.0 ppm for 4 hours -- Female subject 8

Hours	CVen	CTCOH	CBldTCA	zAUrntTCA	AUrnTCOGTCOH	TotCTCOH	CDCVG_Mole
0.5	0.55	nan	0.47	nan	nan	nan	0.0032
1.0	0.81	0.39	1.05	nan	nan	0.39	0.00868

2.0	1.30	1.20	2.73	0.29	4.52	1.20	0.0106
3.0	1.37	1.59	3.85	nan	nan	1.59	0.0127
4.0	1.43	1.93	4.82	nan	nan	1.93	0.0133
4.25	0.81	1.97	5.02	nan	nan	1.97	0.0087
4.5	0.54	1.75	5.29	1.62	8.37	1.75	0.00508
5.0	0.35	1.63	5.37	2.09	12.49	1.63	0.00229
6.0	0.18	1.32	6.01	4.01	19.46	1.32	0.00074
8.0	nan	1.10	7.60	5.81	29.26	1.10	nan
10.0	nan	0.91	6.77	8.27	35.93	0.91	nan
12.0	nan	nan	nan	10.21	40.21	nan	nan
14.0	nan	0.83	8.65	13.06	44.90	0.83	nan
16.0	nan	nan	nan	16.29	48.15	nan	nan
18.0	nan	0.69	9.49	19.09	51.04	0.69	nan
20.0	nan	nan	nan	21.96	55.72	nan	nan
22.0	nan	0.54	10.64	24.17	58.76	0.54	nan
25.0	nan	nan	nan	27.09	60.75	nan	nan
29.25	nan	nan	nan	29.05	62.24	nan	nan
32.5	nan	nan	nan	35.13	72.07	nan	nan
36.0	nan	nan	nan	45.84	76.15	nan	nan
38.25	nan	nan	nan	56.12	79.24	nan	nan
41.0	nan	nan	nan	65.21	81.48	nan	nan
45.0	nan	nan	nan	75.98	83.84	nan	nan
46.0	nan	nan	9.58	nan	nan	nan	nan
49.0	nan	nan	nan	81.05	86.37	nan	nan
50.25	nan	nan	nan	83.74	87.44	nan	nan
53.75	nan	nan	nan	87.89	88.84	nan	nan
56.25	nan	nan	nan	91.72	90.90	nan	nan
59.25	nan	nan	nan	97.13	92.91	nan	nan
67.0	nan	nan	nan	100.34	94.07	nan	nan
73.25	nan	nan	nan	102.88	94.96	nan	nan
75.75	nan	nan	8.55	nan	nan	nan	nan
80.5	nan	nan	nan	106.50	96.17	nan	nan
83.5	nan	nan	nan	110.02	96.82	nan	nan
86.0	nan	nan	nan	113.61	97.41	nan	nan
93.0	nan	nan	nan	117.51	98.54	nan	nan
94.25	nan	nan	7.82	nan	nan	nan	nan

Kimmerle and Eben, 1973

TCE Inhalation 40.0 ppm for 4 hours – female #1

Hours	CVen	CTCOH	AUrnTCOGTCOH	zAUrnTCA	AUrnTCOGTCOH_Coll	zAUrnTCA_Coll
4.0	0.196	0.706	12.046	1.32	nan	nan
5.0	0.104	0.693	nan	nan	nan	nan
6.0	0.078	0.614	nan	nan	nan	nan
7.0	nan	0.574	nan	nan	nan	nan
8.0	nan	0.602	15.644	1.645	nan	nan
24.0	nan	0.473	41.741	5.803	nan	nan
48.0	nan	0.244	61.959	18.403	nan	nan
72.0	nan	0.200	75.097	32.335	nan	nan
96.0	nan	nan	81.615	40.805	nan	nan
120.0	nan	nan	85.263	48.605	nan	nan
192.0	nan	nan	nan	nan	1.297	2.322

TCE Inhalation 44.0 ppm for 4 hours – female #1

Hours	CVen	CTCOH	AUrnTCOGTCOH	zAUrnTCA	AUrnTCOGTCOH_Coll	zAUrnTCA_Coll
4.0	0.479	1.636	8.816	0.294	nan	nan
5.0	0.151	1.621	nan	nan	nan	nan
6.0	0.109	1.335	nan	nan	nan	nan
7.0	0.077	1.195	nan	nan	nan	nan
8.0	nan	1.302	24.940	1.842	nan	nan
24.0	nan	0.525	44.218	7.027	nan	nan
32.0	nan	0.659	nan	nan	nan	nan
48.0	nan	0.134	60.919	19.845	nan	nan
72.0	nan	0.096	68.921	31.698	nan	nan
96.0	nan	nan	70.903	38.408	nan	nan
192.0	nan	nan	nan	nan	0.239	3.682

TCE Inhalation 44.0 ppm for 4 hours – female #3

Hours, CVen, CTCOH, AUrnTCOGTCOH, zAUrnTCA, AUrnTCOGTCOH_Coll, zAUrnTCA_Coll

4.0	0.277	1.776	23.797	0.467	nan	nan
5.0	0.216	1.712	nan	nan	nan	nan
6.0	0.113	1.465	nan	nan	nan	nan
7.0	0.077	1.320	nan	nan	nan	nan
8.0	nan	1.545	28.703	1.333	nan	nan
24.0	nan	0.521	58.809	14.093	nan	nan
32.0	nan	0.543	nan	nan	nan	nan
48.0	nan	0.108	85.586	30.235	nan	nan
72.0	nan	0.050	93.276	42.643	nan	nan
96.0	nan	nan	95.967	51.288	nan	nan
192.0	nan	nan	nan	nan	0.268	1.518

TCE Inhalation 44.0 ppm for 4 hours – female #4

Hours,	CVen,	CTCOH,	AUrnTCOGTCOH,	zAUrnTCA,	AUrnTCOGTCOH_Coll,	zAUrnTCA_Coll
4.0	0.322	0.775	6.262	0.426	nan	nan
5.0	0.117	0.660	nan	nan	nan	nan
6.0	0.117	0.638	nan	nan	nan	nan
7.0	nan	0.585	nan	nan	nan	nan
8.0	nan	0.574	15.150	1.195	nan	nan
24.0	nan	0.438	29.190	6.565	nan	nan
48.0	nan	0.200	36.782	11.965	nan	nan
72.0	nan	0.141	42.539	23.235	nan	nan
96.0	nan	nan	44.553	32.775	nan	nan
120.0	nan	nan	46.221	37.960	nan	nan
192.0	nan	nan	nan	nan	1.126	1.28

TCE Inhalation 40.0 ppm for 4 hours – male #1

Hours,	CVen,	CTCOH,	AUrnTCOGTCOH,	zAUrnTCA,	AUrnTCOGTCOH_Coll,	zAUrnTCA_Coll
4.0	0.252	0.806	12.878	0.205	nan	nan
5.0	0.132	0.681	nan	nan	nan	nan
6.0	0.080	0.614	nan	nan	nan	nan
7.0	nan	0.551	nan	nan	nan	nan
8.0	nan	0.504	24.712	0.489	nan	nan
24.0	nan	0.243	58.083	4.818	nan	nan
48.0	nan	0.080	72.720	17.241	nan	nan
72.0	nan	nan	76.400	28.511	nan	nan
96.0	nan	nan	77.744	38.051	nan	nan
120.0	nan	nan	78.599	43.199	nan	nan
192.0	nan	nan	nan	nan	0.297	2.695

TCE Inhalation 40.0 ppm for 4 hours – male #2

Hours,	CVen,	CTCOH,	AUrnTCOGTCOH,	zAUrnTCA,	AUrnTCOGTCOH_Coll,	zAUrnTCA_Coll
4.0	0.266	0.939	15.053	0.462	nan	nan
5.0	0.127	0.690	nan	nan	nan	nan
6.0	0.078	0.812	nan	nan	nan	nan
7.0	nan	0.696	nan	nan	nan	nan
8.0	nan	0.658	21.897	0.822	nan	nan
24.0	nan	0.339	62.789	8.420	nan	nan
48.0	nan	0.128	85.280	19.045	nan	nan
72.0	nan	0.090	93.302	27.681	nan	nan
96.0	nan	nan	95.789	33.457	nan	nan
120.0	nan	nan	97.177	39.762	nan	nan
192.0	nan	nan	nan	nan	0.324	3.61

TCE Inhalation 44.0 ppm for 4 hours – male #3

Hours,	CVen,	CTCOH,	AUrnTCOGTCOH,	zAUrnTCA,	AUrnTCOGTCOH_Coll,	zAUrnTCA_Coll
4.0	0.246	1.323	11.722	nan	nan	nan
5.0	0.131	1.283	nan	nan	nan	nan
6.0	0.077	1.191	nan	nan	nan	nan
7.0	0.077	1.035	nan	nan	nan	nan
8.0	nan	1.093	37.419	0.585	nan	nan
24.0	nan	0.551	92.855	4.673	nan	nan
32.0	nan	0.403	nan	nan	nan	nan
48.0	nan	0.155	114.296	11.492	nan	nan
72.0	nan	0.098	121.185	18.063	nan	nan
96.0	nan	0.044	123.768	23.734	nan	nan
192.0	nan	nan	nan	nan	0.234	2.108

TCE Repeated Inhalation 48.0 ppm for 4 hours/day for 5 days – subject #1

Hours	CVen	CTCOH	AUrnTCOGTCOH	zAUrnTCA	AUrnTCOGTCOH_Coll	zAUrnTCA_Coll
4.0	0.42	2.047	nan	nan	nan	nan
5.0	0.13	1.672	nan	nan	nan	nan
8.0	0.085	1.596	nan	nan	nan	nan
9.0	nan	1.406	nan	nan	nan	nan
10.0	nan	1.26	nan	nan	nan	nan
24.0	nan	1.174	46.14	4.175	nan	nan
28.0	0.51	2.002	nan	nan	nan	nan
33.0	0.17	1.801	nan	nan	nan	nan
48.0	nan	0.917	121.6	19.16	nan	nan
52.0	0.408	2.38	nan	nan	nan	nan
57.0	nan	1.72	nan	nan	nan	nan
72.0	nan	0.946	175.55	46.72	nan	nan
76.0	0.51	2.58	nan	nan	nan	nan
81.0	nan	2.064	nan	nan	nan	nan
96.0	nan	1.267	nan	238.17	72.82	nan
100.0	nan	2.509	nan	nan	nan	nan
104.0	nan	2.142	nan	nan	nan	nan
105.0	nan	2.116	nan	nan	nan	nan
120.0	nan	2.110	nan	358.26	124.285	nan
144.0	nan	0.507	nan	378.55	153.321	nan
168.0	nan	0.272	nan	396.33	168.271	nan
192.0	nan	0.138	nan	nan	nan	nan
216.0	nan	0.080	nan	nan	nan	nan
240.0	nan	0.054	nan	nan	nan	nan
264.0	nan	0.030	nan	nan	nan	nan
408.0	nan	nan	nan	nan	0.2	1.365

TCE Repeated Inhalation 48.0 ppm for 4 hours/day for 5 days – subject #2

Hours	CVen	CTCOH	AUrnTCOGTCOH	zAUrnTCA	AUrnTCOGTCOH_Coll	zAUrnTCA_Coll
4.0	0.340	1.958	nan	nan	nan	nan
5.0	0.230	1.596	nan	nan	nan	nan
8.0	0.130	1.368	nan	nan	nan	nan
9.0	nan	1.204	nan	nan	nan	nan
10.0	nan	1.152	nan	nan	nan	nan
24.0	nan	1.036	88.46	6.613	nan	nan
28.0	0.340	1.820	nan	nan	nan	nan
33.0	nan	1.674	nan	nan	nan	nan
48.0	nan	0.812	214.54	25.399	nan	nan
52.0	0.476	2.01	nan	nan	nan	nan
57.0	nan	1.87	nan	nan	nan	nan
72.0	nan	0.591	335.72	75.391	nan	nan
76.0	0.272	2.322	nan	nan	nan	nan
81.0	nan	1.909	nan	nan	nan	nan
96.0	nan	0.845	453.37	139.375	nan	nan
100.0	nan	2.509	nan	nan	nan	nan
104.0	nan	2.016	nan	nan	nan	nan
105.0	nan	2.016	nan	nan	nan	nan
120.0	nan	1.010	557.89	229.037	nan	nan
144.0	nan	0.386	600.50	271.661	nan	nan
168.0	nan	0.102	638.16	304.179	nan	nan
192.0	nan	nan	643.27	328.651	nan	nan
216.0	nan	0.040	647.10	346.571	nan	nan
240.0	nan	nan	649.13	360.221	nan	nan
264.0	nan	nan	650.17	371.781	nan	nan
408.0	nan	nan	nan	nan	0.08	2.1

TCE Repeated Inhalation 48.0 ppm for 4 hours/day for 5 days – subject #3

Hours	CVen	CTCOH	AUrnTCOGTCOH	zAUrnTCA	AUrnTCOGTCOH_Coll	zAUrnTCA_Coll
4.0	0.28	1.275	nan	nan	nan	nan
5.0	1.18	1.014	nan	nan	nan	nan
8.0	0.09	0.900	nan	nan	nan	nan
9.0	nan	0.803	nan	nan	nan	nan
10.0	nan	0.720	nan	nan	nan	nan
24.0	nan	0.567	63.33	5.341	nan	nan
28.0	0.34	1.44	nan	nan	nan	nan

33.0	nan	1.85	nan	nan	nan	nan
48.0	nan	0.55	149.89	17.631	nan	nan
52.0	0.34	2.09	nan	nan	nan	nan
57.0	nan	1.40	nan	nan	nan	nan
72.0	nan	0.676	234.33	49.311	nan	nan
76.0	0.34	1.565	nan	nan	nan	nan
81.0	nan	1.248	nan	nan	nan	nan
96.0	nan	0.507	320.33	110.463	nan	nan
100.0	nan	1.974	nan	nan	nan	nan
104.0	nan	1.638	nan	nan	nan	nan
105.0	nan	1.323	nan	nan	nan	nan
120.0	nan	0.510	409.94	187.167	nan	nan
144.0	nan	0.179	434.46	234.983	nan	nan
168.0	nan	nan	440.59	283.309	nan	nan
192.0	nan	0.045	444.02	319.077	nan	nan
216.0	nan	0.028	446.58	337.788	nan	nan
240.0	nan	nan	447.90	356.118	nan	nan
264.0	nan	nan	448.61	372.468	nan	nan
408.0	nan	nan	nan	nan	0.07	2.184

TCE Repeated Inhalation 48.0 ppm for 4 hours/day for 5 days – subject #4

Hours,	CVen,	CTCOH,	AUrnTCOGTCOH,	zAUrnTCA,	zAUrnTCA_Coll
4.0	0.170	2.849	nan	nan	nan
5.0	0.170	2.394	nan	nan	nan
8.0	0.090	2.280	nan	nan	nan
9.0	nan	2.052	nan	nan	nan
10.0	nan	1.976	nan	nan	nan
24.0	nan	1.296	116.10	2.928	nan
28.0	0.340	2.912	nan	nan	nan
33.0	nan	2.429	nan	nan	nan
48.0	nan	0.825	246.68	12.19	nan
52.0	0.272	2.530	nan	nan	nan
57.0	nan	2.260	nan	nan	nan
72.0	nan	0.473	363.79	29.482	nan
76.0	nan	2.322	nan	nan	nan
81.0	nan	2.418	nan	nan	nan
96.0	nan	0.760	458.92	48.094	nan
100.0	nan	2.870	nan	nan	nan
104.0	nan	2.520	nan	nan	nan
105.0	nan	2.293	nan	nan	nan
120.0	nan	1.010	556.48	111.934	nan
144.0	nan	0.198	597.53	169.81	nan
168.0	nan	0.034	638.45	186.895	nan
192.0	nan	nan	641.52	206.764	nan
216.0	nan	nan	642.45	218.839	nan
240.0	nan	nan	642.84	230.578	nan
264.0	nan	nan	642.97	239.119	nan
408.0	nan	nan	nan	nan	3.564

Monster et al., 1976

Data were truncated in EPA (2011) file -- individual data were not presented in Monster et al. (1976) so only the missing points were digitized from the figures in EPA (2011)

TCE Inhalation 65.0 ppm for 4 hours – subject 1

Hours,	RetDose,	CAlvPPM,	CVen,	TotCTCOH,	CBldTCA,	AUrnTCOGTCOH,	zAUrnTCA
3.5	nan	nan	1.2	4.3	3.6	nan	nan
4.0	320.0	nan	nan	nan	nan	nan	nan
4.5	nan	3.766118721	nan	nan	nan	nan	nan
6.0	nan	1.842123288	0.13	4.4	5.7	nan	nan
16.0	nan	nan	nan	nan	nan	31.5445	1.1445
24.0	nan	0.122808219	0.01	1.1	10.1	84.4675	3.27
32.0	nan	nan	nan	nan	nan	119.4505	5.232
40.0	nan	nan	nan	nan	nan	146.3605	8.502
48.0	nan	0.034795662	nan	nan	11.4	157.573	9.9735
56.0	nan	nan	nan	nan	nan	163.553	10.791
64.0	nan	nan	nan	nan	nan	169.0845	12.099
72.0	nan	0.020877397	nan	nan	11.8	176.709	14.388
80.0	nan	nan	nan	nan	nan	175.1657	15.5325

88.0	nan	nan	nan	nan	nan	182.7512	16.8405

TCE Inhalation 140.0 ppm for 4 hours – subject 1

Hours	RetDose	CAlvPPM	CVen	TotCTCOH	CBldTCA	AUrnTCOGTCOH	zAUrnTCA
4.0	740.0	nan	nan	6.1	5.2	nan	nan
4.5	nan	5.989968911	nan	nan	nan	nan	nan
6.5	nan	2.572163121	0.28	7.2	9.0	nan	nan
16.0	nan	nan	nan	nan	nan	58.305	0.8175
24.0	nan	0.28188089	0.014	2.9	15.0	164.5995	3.597
32.0	nan	nan	nan	nan	nan	246.675	5.559
40.0	nan	nan	nan	nan	nan	295.113	9.81
48.0	nan	0.070470222	0.005	0.72	20.0	326.209	13.8975
56.0	nan	nan	nan	nan	nan	340.561	17.1675
64.0	nan	nan	nan	nan	nan	353.418	22.563
72.0	nan	nan	0.0025	0.15	17.5	360.594	26.9775
80.0	nan	nan	nan	nan	nan	364.481	28.9395
142.0	nan	nan	nan	nan	12.5	nan	nan
214.0	nan	nan	nan	nan	7.4	nan	nan
479.0	nan	nan	nan	nan	1.5	nan	nan

TCE Inhalation 68.0 ppm for 4 hours – subject 2

Hours	RetDose	CAlvPPM	CVen	TotCTCOH	CBldTCA	AUrnTCOGTCOH	zAUrnTCA
3.5	nan	nan	1.5	2.9	4.0	nan	nan
4.0	430.0	3.675658588	nan	nan	nan	nan	nan
4.5	nan	1.531524412	nan	nan	nan	nan	nan
6.0	nan	nan	0.16	2.5	6.6	nan	nan
8.0	nan	nan	nan	nan	nan	nan	0.4905
16.0	nan	nan	nan	nan	nan	41.86	2.1255
22.0	nan	0.245043906	0.0156	0.45	9.1	nan	nan
24.0	nan	nan	nan	nan	nan	92.391	7.0305
32.0	nan	nan	nan	nan	nan	117.507	11.9355
40.0	nan	nan	nan	nan	nan	136.4935	19.7835
48.0	nan	0.110269758	0.0065	0.15	8.9	148.1545	25.3425
56.0	nan	nan	nan	nan	nan	155.6295	29.103
64.0	nan	nan	nan	nan	nan	162.5065	34.989
72.0	nan	nan	0.0034	nan	8.8	169.52729	41.856
80.0	nan	0.076882525	nan	nan	nan	174.51315	46.2705
88.0	nan	nan	nan	nan	nan	181.89123	51.5025
142.0	nan	nan	nan	nan	4.5	nan	nan
214.0	nan	nan	nan	nan	2.4	nan	nan

TCE Inhalation 138.0 ppm for 4 hours – subject 2

Hours	RetDose	CAlvPPM	CVen	TotCTCOH	CBldTCA	AUrnTCOGTCOH	zAUrnTCA
4.0	790.0	4.993960819	nan	4.5	4.0	nan	nan
6.0	nan	3.433348063	0.22	3.9	6.6	nan	nan
16.0	nan	nan	nan	nan	nan	74.75	1.7985
24.0	nan	0.343334806	0.028	1.2	12.0	181.493	8.829
32.0	nan	nan	nan	nan	nan	232.7715	14.715
40.0	nan	nan	nan	nan	nan	272.09	26.487
48.0	nan	nan	0.0085	0.35	13.0	301.99	39.24
56.0	nan	0.103000442	nan	nan	nan	315.445	47.415
64.0	nan	nan	nan	nan	nan	324.415	55.59
72.0	nan	nan	0.0048	0.11	11.0	331.292	64.419
80.0	nan	nan	nan	nan	nan	336.076	71.1225
95.0	nan	0.043697157	0.0011	0.03	10.0	nan	nan
164.0	nan	nan	nan	nan	5.4	nan	nan
260.0	nan	nan	nan	nan	1.6	nan	nan
404.0	nan	nan	nan	nan	0.04	nan	nan

TCE Inhalation 70.0 ppm for 4 hours – subject 3

Hours	RetDose	CAlvPPM	CVen	TotCTCOH	CBldTCA	AUrnTCOGTCOH	zAUrnTCA
4.0	330.0	nan	1.6	2.8	3.1	nan	nan
4.5	nan	5.517282574	nan	nan	nan	nan	nan
6.0	nan	3.678188383	0.18	2.7	5.2	nan	nan
16.0	nan	nan	nan	nan	nan	35.88	1.4715
24.0	nan	0.239082245	0.011	0.51	7.8	91.6435	4.7415
32.0	nan	nan	nan	nan	nan	116.909	7.521

40.0	nan	nan	nan	nan	nan	134.849	14.715
48.0	nan	0.062529203	0.0023	nan	8.1	145.1645	20.4375
56.0	nan	nan	nan	nan	nan	149.6495	22.563
64.0	nan	nan	nan	nan	nan	153.088	26.814
72.0	nan	0.018390942	nan	nan	6.2	155.48	31.2285
80.0	nan	nan	nan	nan	nan	156.676	33.354
88.0	nan	nan	nan	nan	nan	155.47549	36.1335
134.0	nan	nan	nan	nan	4.1	nan	nan
214.0	nan	nan	nan	nan	2.1	nan	nan
454.0	nan	nan	nan	nan	0.04	nan	nan

TCE Inhalation 142.0 ppm for 4 hours – subject 3

Hours,	RetDose,	CAlvPPM,	CVen,	TotCTCOH,	CBldTCA,	AUrnTCOGTCOH,	zAUrnTCA
4.0	710.0	nan	nan	5.2	3.6	nan	nan
4.5	nan	4.884417808	nan	nan	nan	nan	nan
6.0	nan	2.767836758	0.25	5.1	6.5	nan	nan
16.0	nan	nan	nan	nan	nan	49.933	0.654
24.0	nan	0.325627854	0.022	1.6	12.0	132.457	2.4525
32.0	nan	nan	nan	nan	nan	178.204	4.251
40.0	nan	nan	nan	nan	nan	210.3465	11.118
48.0	nan	0.11071347	0.0054	0.34	11.0	226.7915	15.696
56.0	nan	nan	nan	nan	nan	239.499	22.7265
64.0	nan	nan	nan	nan	nan	242.19	25.3425
72.0	nan	0.035819064	0.0025	0.06	10.0	247.871	31.2285
80.0	nan	nan	nan	nan	nan	250.861	36.297
88.0	nan	nan	nan	nan	nan	249.38647	41.202
96.0	nan	nan	nan	nan	nan	249.38647	45.6165
104.0	nan	nan	nan	nan	nan	249.38647	46.83776
191.0	nan	nan	nan	nan	5.8	nan	nan
263.0	nan	nan	nan	nan	3.8	nan	nan
407.0	nan	nan	nan	nan	1.5	nan	nan

TCE Inhalation 76.0 ppm for 4 hours – subject 4

Hours,	RetDose,	CAlvPPM,	CVen,	TotCTCOH,	CBldTCA,	AUrnTCOGTCOH,	zAUrnTCA
4.0	470.0	nan	nan	3.2	2.4	nan	nan
4.5	nan	4.666913489	nan	nan	nan	nan	nan
6.0	nan	2.10011107	0.175	3.2	4.5	nan	nan
16.0	nan	nan	nan	nan	nan	49.7835	1.308
24.0	nan	0.204177465	0.0088	0.6	9.0	121.5435	3.27
32.0	nan	nan	nan	nan	nan	153.088	5.886
40.0	nan	nan	nan	nan	nan	179.5495	12.9165
48.0	nan	0.06125324	0.0025	0.11	11.6	192.257	21.582
56.0	nan	nan	nan	nan	nan	198.237	25.6695
64.0	nan	nan	nan	nan	nan	202.124	30.2475
72.0	nan	0.020417747	nan	nan	9.8	207.3565	35.316
80.0	nan	nan	nan	nan	nan	208.46545	39.4035
88.0	nan	nan	nan	nan	nan	210.65106	44.799
96.0	nan	nan	nan	nan	nan	204.58835	51.339
142.0	nan	nan	nan	nan	5.4	nan	nan
214.0	nan	nan	nan	nan	2.6	nan	nan
504.0	nan	nan	nan	nan	0.25	nan	nan

TCE Inhalation 140.0 ppm for 4 hours – subject 3

Hours,	RetDose,	CAlvPPM,	CVen,	TotCTCOH,	CBldTCA,	AUrnTCOGTCOH,	zAUrnTCA
4.0	790.0	nan	3.1	5.0	3.3	nan	nan
4.5	nan	4.520886183	nan	nan	nan	nan	nan
6.0	nan	2.542998478	0.26	5.5	6.4	nan	nan
16.0	nan	nan	nan	nan	nan	74.75	1.635
24.0	nan	0.268427617	0.019	1.7	11.0	222.755	8.829
32.0	nan	nan	nan	nan	nan	290.7775	17.004
40.0	nan	nan	nan	nan	nan	332.6375	25.6695
48.0	nan	0.062162185	0.004	0.35	14.0	355.0625	40.548
56.0	nan	nan	nan	nan	nan	366.1255	49.8675
64.0	nan	nan	nan	nan	nan	365.36303	60.168
72.0	nan	0.025429985	0.002	0.06	12.5	376.97374	74.229
80.0	nan	nan	nan	nan	nan	373.06307	80.9325
88.0	nan	nan	nan	nan	nan	369.19298	89.271
96.0	nan	nan	nan	nan	nan	365.36303	102.3078

104.0	nan	nan	nan	nan	nan	369.19298	106.46256
144.0	nan	nan	nan	nan	5.3	nan	nan
216.0	nan	nan	nan	nan	3.4	nan	nan

Muller et al., 1974

TCA Oral Gavage 2.646 mg/kg

Hours,	CPlasTCA,	zAUrnTCA
0.5	22.7	nan
1.0	29.4	nan
3.0	23.0	nan
5.5	24.4	nan
10.0	21.8	nan
24.0	17.2	43.4
34.0	15.6	nan
48.0	14.0	59.7
58.0	11.4	nan
72.0	8.95	75.0
82.0	8.48	nan
96.0	5.40	88.7
106.0	5.82	nan
120.0	5.00	98.58
144.0	nan	107.98
168.0	nan	113.03

TCOH Oral Gavage 10.0 mg/kg

Hours,	CTCOH,	AUrnTCOGTCOH,	CPlasTCA,	zAUrnTCA
0.4	5.79	nan	nan	nan
0.5	4.93	nan	4.8	nan
1.0	4.1	nan	3.88	nan
1.5	3.76	nan	6.57	nan
3.0	2.58	nan	nan	nan
3.5	nan	nan	6.86	nan
6.0	1.91	nan	11.5	nan
11.0	1.22	nan	18.7	nan
24.0	0.498	84.2	24.2	27.8
35.0	0.276	nan	20.8	nan
48.0	0.163	100.90	17.1	70.2
72.0	0.0487	109.26	12.1	101.0
96.0	0.0196	113.16	9.28	125.8
120.0	nan	115.39	nan	147.9
122.0	nan	nan	8.72	nan
144.0	nan	nan	5.73	156.74
168.0	nan	nan	5.30	161.23

Paykoc and Powell, 1945

TCA IV 24.8 mg/kg

Hours,	CBldTCA,	CPlasTCA
34.0	65.0	119.0
58.0	50.0	95.0
82.0	44.0	83.0
106.0	32.0	61.0

TCA IV 32.9 mg/kg

Hours,	CBldTCA,	CPlasTCA,	zAUrnTCA
10.0	80.0	140.0	189.0
34.0	57.0	100.0	453.0
58.0	44.0	77.0	703.0
82.0	35.0	61.0	928.0
106.0	28.0	50.0	1075.0
130.0	24.0	42.0	1148.0
154.0	21.0	37.0	1224.0
178.0	nan	nan	1284.0
202.0	nan	nan	1332.0

TCA Oral Gavage 53.06 mg/kg

Hours,	CBldTCA,	CPlasTCA,	zAUrnTCA
34.0	102.0	179.0	900.0
58.0	78.0	136.0	1260.0
82.0	62.0	108.0	1500.0
106.0	48.0	84.0	1690.0
130.0	40.0	70.0	1816.0
154.0	nan	nan	1856.0
178.0	nan	nan	1878.0
202.0	nan	nan	1932.0

APPENDIX K. M FILE FOR MOUSE SENSITIVITY ANALYSIS

The following is an m file for generating output for the mouse sensitivity analysis.

Mouse_SARun.m

```
load @format=model @file=EPA_2011_TCE

Init
ResetDoses
Mouse
CONC=100.0; TCHNG=7.0; DAYS=5.0; TMAX=1680.0; TSTP=1680.0; DOSEINT=24.0; AVGINT=168.0;
SA_All
SA_Rodent
SA_Mouse
save sasum_hours @file='mouse_saresults_hours1.txt' @format=ascii
save sasum_auccblddm @file='mouse_saresults_auccblddm1.txt' @format=ascii
save sasum_auclivtcadm @file='mouse_saresults_auclivtcadm1.txt' @format=ascii
save sasum_aucctcohdm @file='mouse_saresults_aucctcohdm1.txt' @format=ascii
save sasum_auccblddm2 @file='mouse_saresults_auccblddm1b.txt' @format=ascii
save sasum_auclivtcadm2 @file='mouse_saresults_auclivtcadm1b.txt' @format=ascii
save sasum_aucctcohdm2 @file='mouse_saresults_aucctcohdm1b.txt' @format=ascii

ResetDoses
Mouse
CONC=600.0; TCHNG=7.0; DAYS=5.0; TMAX=1680.0; TSTP=1680.0; DOSEINT=24.0; AVGINT=168.0;
SA_All
SA_Rodent
SA_Mouse
save sasum_hours @file='mouse_saresults_hours2.txt' @format=ascii
save sasum_auccblddm @file='mouse_saresults_auccblddm2.txt' @format=ascii
save sasum_auclivtcadm @file='mouse_saresults_auclivtcadm2.txt' @format=ascii
save sasum_aucctcohdm @file='mouse_saresults_aucctcohdm2.txt' @format=ascii
save sasum_auccblddm2 @file='mouse_saresults_auccblddm2b.txt' @format=ascii
save sasum_auclivtcadm2 @file='mouse_saresults_auclivtcadm2b.txt' @format=ascii
save sasum_aucctcohdm2 @file='mouse_saresults_aucctcohdm2b.txt' @format=ascii

ResetDoses
Mouse
PDOSE=300.0; TCHNG=0.05; DAYS=5.0; TMAX=1680.0; TSTP=1680.0; DOSEINT=24.0; AVGINT=168.0;
SA_All
SA_Rodent
SA_Mouse
SA_OralGav
save sasum_hours @file='mouse_saresults_hours3.txt' @format=ascii
save sasum_auccblddm @file='mouse_saresults_auccblddm3.txt' @format=ascii
save sasum_auclivtcadm @file='mouse_saresults_auclivtcadm3.txt' @format=ascii
save sasum_aucctcohdm @file='mouse_saresults_aucctcohdm3.txt' @format=ascii
save sasum_auccblddm2 @file='mouse_saresults_auccblddm3b.txt' @format=ascii
save sasum_auclivtcadm2 @file='mouse_saresults_auclivtcadm3b.txt' @format=ascii
save sasum_aucctcohdm2 @file='mouse_saresults_aucctcohdm3b.txt' @format=ascii

ResetDoses
Mouse
PDOSE=1000.0; TCHNG=0.05; DAYS=5.0; TMAX=1680.0; TSTP=1680.0; DOSEINT=24.0; AVGINT=168.0;
SA_All
SA_Rodent
SA_Mouse
SA_OralGav
save sasum_hours @file='mouse_saresults_hours4.txt' @format=ascii
save sasum_auccblddm @file='mouse_saresults_auccblddm4.txt' @format=ascii
save sasum_auclivtcadm @file='mouse_saresults_auclivtcadm4.txt' @format=ascii
save sasum_aucctcohdm @file='mouse_saresults_aucctcohdm4.txt' @format=ascii
save sasum_auccblddm2 @file='mouse_saresults_auccblddm4b.txt' @format=ascii
save sasum_auclivtcadm2 @file='mouse_saresults_auclivtcadm4b.txt' @format=ascii
save sasum_aucctcohdm2 @file='mouse_saresults_aucctcohdm4b.txt' @format=asci
```

APPENDIX L. M FILE FOR RAT SENSITIVITY ANALYSIS

The following is an m file for generating output for the rat sensitivity analysis.

Rat_SARun.m

```
load @format=model @file=EPA_2011_TCE

Init
ResetDoses
Rat
CONC=100.0; TCHNG=7.0; DAYS=5.0; TMAX=1680.0; TSTP=1680.0; DOSEINT=24.0; AVGINT=168.0;
SA_All
SA_Rodent
save sasum_hours @file='rat_saresults_hours1.txt' @format=ascii
save sasum_auccblddm @file='rat_saresults_auccblddm1.txt' @format=ascii
save sasum_auclivtcadm @file='rat_saresults_auclivtcadm1.txt' @format=ascii
save sasum_aucctcohdm @file='rat_saresults_aucctcohdm1.txt' @format=ascii
save sasum_auccblddm2 @file='rat_saresults_auccblddm1b.txt' @format=ascii
save sasum_auclivtcadm2 @file='rat_saresults_auclivtcadm1b.txt' @format=ascii
save sasum_aucctcohdm2 @file='rat_saresults_aucctcohdm1b.txt' @format=ascii

ResetDoses
Rat
CONC=600.0; TCHNG=7.0; DAYS=5.0; TMAX=1680.0; TSTP=1680.0; DOSEINT=24.0; AVGINT=168.0;
SA_All
SA_Rodent
save sasum_hours @file='rat_saresults_hours2.txt' @format=ascii
save sasum_auccblddm @file='rat_saresults_auccblddm2.txt' @format=ascii
save sasum_auclivtcadm @file='rat_saresults_auclivtcadm2.txt' @format=ascii
save sasum_aucctcohdm @file='rat_saresults_aucctcohdm2.txt' @format=ascii
save sasum_auccblddm2 @file='rat_saresults_auccblddm2b.txt' @format=ascii
save sasum_auclivtcadm2 @file='rat_saresults_auclivtcadm2b.txt' @format=ascii
save sasum_aucctcohdm2 @file='rat_saresults_aucctcohdm2b.txt' @format=ascii

ResetDoses
Rat
PDOSE=300.0; TCHNG=0.05; DAYS=5.0; TMAX=1680.0; TSTP=1680.0; DOSEINT=24.0; AVGINT=168.0;
SA_All
SA_Rodent
SA_OralGav
save sasum_hours @file='rat_saresults_hours3.txt' @format=ascii
save sasum_auccblddm @file='rat_saresults_auccblddm3.txt' @format=ascii
save sasum_auclivtcadm @file='rat_saresults_auclivtcadm3.txt' @format=ascii
save sasum_aucctcohdm @file='rat_saresults_aucctcohdm3.txt' @format=ascii
save sasum_auccblddm2 @file='rat_saresults_auccblddm3b.txt' @format=ascii
save sasum_auclivtcadm2 @file='rat_saresults_auclivtcadm3b.txt' @format=ascii
save sasum_aucctcohdm2 @file='rat_saresults_aucctcohdm3b.txt' @format=ascii

ResetDoses
Rat
PDOSE=1000.0; TCHNG=0.05; DAYS=5.0; TMAX=1680.0; TSTP=1680.0; DOSEINT=24.0; AVGINT=168.0;
SA_All
SA_Rodent
SA_OralGav
save sasum_hours @file='rat_saresults_hours4.txt' @format=ascii
save sasum_auccblddm @file='rat_saresults_auccblddm4.txt' @format=ascii
save sasum_auclivtcadm @file='rat_saresults_auclivtcadm4.txt' @format=ascii
save sasum_aucctcohdm @file='rat_saresults_aucctcohdm4.txt' @format=ascii
save sasum_auccblddm2 @file='rat_saresults_auccblddm4b.txt' @format=ascii
save sasum_auclivtcadm2 @file='rat_saresults_auclivtcadm4b.txt' @format=ascii
save sasum_aucctcohdm2 @file='rat_saresults_aucctcohdm4b.txt' @format=ascii
```

APPENDIX M. M FILES FOR HUMAN SENSITIVITY ANALYSIS

The following are m files for generating output for the human sensitivity analysis.

Female_SARun.m

```
load @format=model @file=EPA_2011_TCE

Init
ResetDoses
Human
FemalePost
CONC=0.001; TCHNG=16800.0; TSTP=16800.0; DOSEINT=100000.0; AVGINT=24.0;
SA_All
SA_Human
save sasum_hours @file='female_saresults_hours1.txt' @format=ascii
save sasum_auccblddm @file='female_saresults_auccblddm1.txt' @format=ascii
save sasum_auclivtcadm @file='female_saresults_auclivtcadm1.txt' @format=ascii
save sasum_aucctcohdm @file='female_saresults_aucctcohdm1.txt' @format=ascii
save sasum_auccblddm2 @file='female_saresults_auccblddm1b.txt' @format=ascii
save sasum_auclivtcadm2 @file='female_saresults_auclivtcadm1b.txt' @format=ascii
save sasum_aucctcohdm2 @file='female_saresults_aucctcohdm1b.txt' @format=ascii

ResetDoses
Human
FemalePost
DRINK=0.001; TSTP=16800.0; DOSEINT=100000.0; AVGINT=24.0;
SA_All
SA_Human
save sasum_hours @file='female_saresults_hours2.txt' @format=ascii
save sasum_auccblddm @file='female_saresults_auccblddm2.txt' @format=ascii
save sasum_auclivtcadm @file='female_saresults_auclivtcadm2.txt' @format=ascii
save sasum_aucctcohdm @file='female_saresults_aucctcohdm2.txt' @format=ascii
save sasum_auccblddm2 @file='female_saresults_auccblddm2b.txt' @format=ascii
save sasum_auclivtcadm2 @file='female_saresults_auclivtcadm2b.txt' @format=ascii
save sasum_aucctcohdm2 @file='female_saresults_aucctcohdm2b.txt' @format=ascii
```

Male_SARun.m

```
load @format=model @file=EPA_2011_TCE

Init
ResetDoses
Human
MalePost
CONC=0.001; TCHNG=16800.0; TSTP=16800.0; DOSEINT=100000.0; AVGINT=24.0;
SA_All
SA_Human
save sasum_hours @file='male_saresults_hours1.txt' @format=ascii
save sasum_auccblddm @file='male_saresults_auccblddm1.txt' @format=ascii
save sasum_auclivtcadm @file='male_saresults_auclivtcadm1.txt' @format=ascii
save sasum_aucctcohdm @file='male_saresults_aucctcohdm1.txt' @format=ascii
save sasum_auccblddm2 @file='male_saresults_auccblddm1b.txt' @format=ascii
save sasum_auclivtcadm2 @file='male_saresults_auclivtcadm1b.txt' @format=ascii
save sasum_aucctcohdm2 @file='male_saresults_aucctcohdm1b.txt' @format=ascii

ResetDoses
Human
MalePost
DRINK=0.001; TSTP=16800.0; DOSEINT=100000.0; AVGINT=24.0;
SA_All
SA_Human
save sasum_hours @file='male_saresults_hours2.txt' @format=ascii
save sasum_auccblddm @file='male_saresults_auccblddm2.txt' @format=ascii
save sasum_auclivtcadm @file='male_saresults_auclivtcadm2.txt' @format=ascii
save sasum_aucctcohdm @file='male_saresults_aucctcohdm2.txt' @format=ascii
save sasum_auccblddm2 @file='male_saresults_auccblddm2b.txt' @format=ascii
save sasum_auclivtcadm2 @file='male_saresults_auclivtcadm2b.txt' @format=ascii
save sasum_aucctcohdm2 @file='male_saresults_aucctcohdm2b.txt' @format=asci
```

APPENDIX N. ADDITIONAL M FILES

The following are m files for generating output for validation figures and sensitivity analysis.

Init.m

```
prepare T HOURS ZAEXHPOST AURNTCOGTCOH AURNTCOGTCOH_COLL AURNTCTOT_MOLE CALVPPM CART CBLDMIX
CBLDTCA CDCVG_MOLE
prepare CFAT CGUT CINHPPM CKID CLIV CLIVTCA CLIVTCOGTCOH CLIVTCOH CMIXEXH CMUS CPLASTCA CSLW
CTCOG CTCOGTCOH CTCOH CVEN
prepare RETDOSE TOTCTCOH ZABILETCOG ZAURNNDCVC ZAURNTCA ZAURNTCA_COLL
prepare AUCCBLD AUCCTCOH AUCLIVTCA

HVDPRN=0;
WESITG=0;
CJVITG=0;
```

ResetDoses.m

```
  CC=0; NRODENTS=1.0; KLOSSC=0.0; VCHC=1.0;
  CONC=0.0; IVDOSE=0.0; TCHNG=1.0; DAYS=1.0; TMAX=24.0;
  PDOSE=0.0; DRINK=0.0; IADOSE=0.0; PVDOSE=0.0;
  IVDOSETCA=0.0; PDOSETCA=0.0;
  IVDOSETCOH=0.0; PDOSETCOH=0.0;
  URNMISSING=0; COLLECTTM=100000.0; COLLECTINT=100000.0;
  CINT=0.01; DOSEINT=100000.0; AVGINT=1.0;
```

SA_Mouse.m

```
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kdcvgcs=[];  cenKDCVGC=KDCVGC;
for KDCVGC=[cenKDCVGC*(1.0-delta) cenKDCVGC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kdcvgcs=[kdcvgcs KDCVGC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KDCVGC=cenKDCVGC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------------finished KDCVGC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  frackiddcvccs=[];
cenFRACKIDDCVCC=FRACKIDDCVCC;
for FRACKIDDCVCC=[cenFRACKIDDCVCC*(1.0-delta) cenFRACKIDDCVCC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  frackiddcvccs=[frackiddcvccs FRACKIDDCVCC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
```

```
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    FRACKIDDCVCC=cenFRACKIDDCVCC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-------------------------------------finished FRACKIDDCVCC");
```

SA_Rodent.m

```
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kmcs=[];  cenKMC=KMC;
for KMC=[cenKMC*(1.0-delta) cenKMC*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms
AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kmcs=[kmcs KMC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KMC=cenKMC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];
    sasum_aucctcohdm=[sasum_aucctcohdm sa_aucctcohdm];
    disp("----------------------------------------------finished KMC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vmaxdcvgcs=[];  cenVMAXDCVGC=VMAXDCVGC;
for VMAXDCVGC=[cenVMAXDCVGC*(1.0-delta) cenVMAXDCVGC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  vmaxdcvgcs=[vmaxdcvgcs VMAXDCVGC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VMAXDCVGC=cenVMAXDCVGC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("----------------------------------------finished VMAXDCVGC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vmaxkiddcvgcs=[];
cenVMAXKIDDCVGC=VMAXKIDDCVGC;
for VMAXKIDDCVGC=[cenVMAXKIDDCVGC*(1.0-delta) cenVMAXKIDDCVGC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  vmaxkiddcvgcs=[vmaxkiddcvgcs VMAXKIDDCVGC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
```

```
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VMAXKIDDCVGC=cenVMAXKIDDCVGC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-------------------------------------finished VMAXKIDDCVGC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vmaxtcohcs=[];  cenVMAXTCOHC=VMAXTCOHC;
for VMAXTCOHC=[cenVMAXTCOHC*(1.0-delta) cenVMAXTCOHC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  vmaxtcohcs=[vmaxtcohcs VMAXTCOHC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VMAXTCOHC=cenVMAXTCOHC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("----------------------------------------finished VMAXTCOHC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vmaxgluccs=[];  cenVMAXGLUCC=VMAXGLUCC;
for VMAXGLUCC=[cenVMAXGLUCC*(1.0-delta) cenVMAXGLUCC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  vmaxgluccs=[vmaxgluccs VMAXGLUCC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VMAXGLUCC=cenVMAXGLUCC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("----------------------------------------finished VMAXGLUCC");
```

SA_Human.m

```
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  cls=[];  cenCL=CL;  for CL=[cenCL*(1.0-delta)
cenCL*(1.0+delta)];
start @NoCallback;  auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];  sasum_hours=[sasum_hours HOURS];  cls=[cls CL];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    CL=cenCL;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];
```

```
    sasum_aucctcohdm=[sasum_aucctcohdm sa_aucctcohdm];
    disp("---------------------------------------------finished CL");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kmdcvgcs=[];  cenKMDCVGC=KMDCVGC;
for KMDCVGC=[cenKMDCVGC*(1.0-delta) cenKMDCVGC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kmdcvgcs=[kmdcvgcs KMDCVGC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KMDCVGC=cenKMDCVGC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("------------------------------------------finished KMDCVGC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kmkiddcvgcs=[];  cenKMKIDDCVGC=KMKIDDCVGC;
for KMKIDDCVGC=[cenKMKIDDCVGC*(1.0-delta) cenKMKIDDCVGC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  kmkiddcvgcs=[kmkiddcvgcs KMKIDDCVGC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KMKIDDCVGC=cenKMKIDDCVGC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------finished KMKIDDCVGC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  cltcohs=[];  cenCLTCOH=CLTCOH;
for CLTCOH=[cenCLTCOH*(1.0-delta) cenCLTCOH*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
cltcohs=[cltcohs CLTCOH];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    CLTCOH=cenCLTCOH;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------------finished CLTCOH");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  clglucs=[];  cenCLGLUC=CLGLUC;
```

```
for CLGLUC=[cenCLGLUC*(1.0-delta) cenCLGLUC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
clglucs=[clglucs CLGLUC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    CLGLUC=cenCLGLUC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished CLGLUC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kdcvgcs=[];  cenKDCVGC=KDCVGC;
for KDCVGC=[cenKDCVGC*(1.0-delta) cenKDCVGC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kdcvgcs=[kdcvgcs KDCVGC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KDCVGC=cenKDCVGC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished KDCVGC");
SA_OralGav.m
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kass=[];  cenKAS=KAS;  for KAS=[cenKAS*(1.0-
delta) cenKAS*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  kass=[kass KAS];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];  sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KAS=cenKAS;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("------------------------------------------------finished KAS");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  ktsds=[];  cenKTSD=KTSD;  for
KTSD=[cenKTSD*(1.0-delta) cenKTSD*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms
AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  ktsds=[ktsds KTSD];  end;
```

```
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];  sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KTSD=cenKTSD;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished KTSD");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kads=[];  cenKAD=KAD;  for KAD=[cenKAD*(1.0-
delta) cenKAD*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  kads=[kads KAD];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];  sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KAD=cenKAD;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("----------------------------------------------finished KAD");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  ktds=[];  cenKTD=KTD;  for KTD=[cenKTD*(1.0-
delta) cenKTD*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  ktds=[ktds KTD];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];  sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KTD=cenKTD;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("----------------------------------------------finished KTD");
```

SA_All.m

```
sasum_auccblddm=[];  sasum_auclivtcadm=[];  sasum_aucctcohdm=[];  sasum_hours=[];  delta=0.1/2.0;
sasum_auccblddm2=[];  sasum_auclivtcadm2=[];  sasum_aucctcohdm2=[];

auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  bws=[];  cenBW=BW;  for BW=[cenBW*(1.0-delta)
cenBW*(1.0+delta)];
start @NoCallback;  auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
    aucctcohdms=[aucctcohdms AUCCTCOHDM];  sasum_hours=[sasum_hours HOURS];  bws=[bws BW];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
```

```
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    BW=cenBW;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];
    sasum_aucctcohdm=[sasum_aucctcohdm sa_aucctcohdm];
    disp("-----------------------------------------------finished BW");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  qccs=[];  cenQCC=QCC;
for QCC=[cenQCC*(1.0-delta) cenQCC*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms
AUCCBLDDM];
    auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
    qccs=[qccs QCC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    QCC=cenQCC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];
    sasum_aucctcohdm=[sasum_aucctcohdm sa_aucctcohdm];
    disp("----------------------------------------------finished QCC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vprs=[];  cenVPR=VPR;
for VPR=[cenVPR*(1.0-delta) cenVPR*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms
AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
vprs=[vprs VPR];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VPR=cenVPR;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];
    sasum_aucctcohdm=[sasum_aucctcohdm sa_aucctcohdm];
    disp("----------------------------------------------finished VPR");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  drespcs=[];  cenDRESPC=DRESPC;
for DRESPC=[cenDRESPC*(1.0-delta) cenDRESPC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
drespcs=[drespcs DRESPC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
```

```
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    DRESPC=cenDRESPC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-------------------------------------------finished DRESPC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  qfatcs=[];  cenQFATC=QFATC;
for QFATC=[cenQFATC*(1.0-delta) cenQFATC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
qfatcs=[qfatcs QFATC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    QFATC=cenQFATC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-------------------------------------------finished QFATC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  qgutcs=[];  cenQGUTC=QGUTC;
for QGUTC=[cenQGUTC*(1.0-delta) cenQGUTC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
qgutcs=[qgutcs QGUTC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    QGUTC=cenQGUTC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-------------------------------------------finished QGUTC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  qkidcs=[];  cenQKIDC=QKIDC;
for QKIDC=[cenQKIDC*(1.0-delta) cenQKIDC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
qkidcs=[qkidcs QKIDC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
```

```
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    QKIDC=cenQKIDC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished QKIDC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  qlivcs=[];  cenQLIVC=QLIVC;
for QLIVC=[cenQLIVC*(1.0-delta) cenQLIVC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
qlivcs=[qlivcs QLIVC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    QLIVC=cenQLIVC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished QLIVC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  qslwcs=[];  cenQSLWC=QSLWC;
for QSLWC=[cenQSLWC*(1.0-delta) cenQSLWC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
qslwcs=[qslwcs QSLWC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    QSLWC=cenQSLWC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished QSLWC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vbldcs=[];  cenVBLDC=VBLDC;
for VBLDC=[cenVBLDC*(1.0-delta) cenVBLDC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
vbldcs=[vbldcs VBLDC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
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    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VBLDC=cenVBLDC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------------finished VBLDC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vfatcs=[];  cenVFATC=VFATC;
for VFATC=[cenVFATC*(1.0-delta) cenVFATC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
vfatcs=[vfatcs VFATC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VFATC=cenVFATC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------------finished VFATC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vgutcs=[];  cenVGUTC=VGUTC;
for VGUTC=[cenVGUTC*(1.0-delta) cenVGUTC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
vgutcs=[vgutcs VGUTC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VGUTC=cenVGUTC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------------finished VGUTC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vkidcs=[];  cenVKIDC=VKIDC;
for VKIDC=[cenVKIDC*(1.0-delta) cenVKIDC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
vkidcs=[vkidcs VKIDC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
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    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VKIDC=cenVKIDC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished VKIDC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vlivcs=[];  cenVLIVC=VLIVC;
for VLIVC=[cenVLIVC*(1.0-delta) cenVLIVC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
vlivcs=[vlivcs VLIVC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VLIVC=cenVLIVC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished VLIVC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vrapcs=[];  cenVRAPC=VRAPC;
for VRAPC=[cenVRAPC*(1.0-delta) cenVRAPC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
vrapcs=[vrapcs VRAPC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VRAPC=cenVRAPC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished VRAPC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vresplumcs=[];  cenVRESPLUMC=VRESPLUMC;
for VRESPLUMC=[cenVRESPLUMC*(1.0-delta) cenVRESPLUMC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  vresplumcs=[vresplumcs VRESPLUMC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VRESPLUMC=cenVRESPLUMC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
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    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------finished VRESPLUMC");
aucbblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vrespcs=[];  cenVRESPC=VRESPC;
for VRESPC=[cenVRESPC*(1.0-delta) cenVRESPC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
vrespcs=[vrespcs VRESPC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VRESPC=cenVRESPC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("------------------------------------------finished VRESPC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vperfcs=[];  cenVPERFC=VPERFC;
for VPERFC=[cenVPERFC*(1.0-delta) cenVPERFC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
vperfcs=[vperfcs VPERFC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VPERFC=cenVPERFC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("------------------------------------------finished VPERFC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  fracplass=[];  cenFRACPLAS=FRACPLAS;
for FRACPLAS=[cenFRACPLAS*(1.0-delta) cenFRACPLAS*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
fracplass=[fracplass FRACPLAS];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    FRACPLAS=cenFRACPLAS;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
```

```
    disp("-----------------------------------------finished FRACPLAS");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  pbs=[];  cenPB=PB;  for PB=[cenPB*(1.0-delta)
cenPB*(1.0+delta)];
start @NoCallback;  auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];  sasum_hours=[sasum_hours HOURS];  pbs=[pbs PB];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PB=cenPB;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];
    sasum_aucctcohdm=[sasum_aucctcohdm sa_aucctcohdm];
    disp("-----------------------------------------------finished PB");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  pfats=[];  cenPFAT=PFAT;
for PFAT=[cenPFAT*(1.0-delta) cenPFAT*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms
AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
pfats=[pfats PFAT];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PFAT=cenPFAT;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished PFAT");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  pguts=[];  cenPGUT=PGUT;
for PGUT=[cenPGUT*(1.0-delta) cenPGUT*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms
AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
pguts=[pguts PGUT];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PGUT=cenPGUT;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished PGUT");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  pkids=[];  cenPKID=PKID;
for PKID=[cenPKID*(1.0-delta) cenPKID*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms
AUCCBLDDM];
```

```
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
pkids=[pkids PKID];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PKID=cenPKID;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished PKID");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  plivs=[];  cenPLIV=PLIV;
for PLIV=[cenPLIV*(1.0-delta) cenPLIV*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms
AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
plivs=[plivs PLIV];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PLIV=cenPLIV;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished PLIV");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  praps=[];  cenPRAP=PRAP;
for PRAP=[cenPRAP*(1.0-delta) cenPRAP*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms
AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
praps=[praps PRAP];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PRAP=cenPRAP;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished PRAP");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  presps=[];  cenPRESP=PRESP;
for PRESP=[cenPRESP*(1.0-delta) cenPRESP*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
```

```
presps=[presps PRESP];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PRESP=cenPRESP;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished PRESP");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  pslws=[];  cenPSLW=PSLW;
for PSLW=[cenPSLW*(1.0-delta) cenPSLW*(1.0+delta)];  start @NoCallback;  auccblddms=[auccblddms
AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
pslws=[pslws PSLW];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PSLW=cenPSLW;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("----------------------------------------------finished PSLW");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  prbcplastcas=[];  cenPRBCPLASTCA=PRBCPLASTCA;
for PRBCPLASTCA=[cenPRBCPLASTCA*(1.0-delta) cenPRBCPLASTCA*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  prbcplastcas=[prbcplastcas PRBCPLASTCA];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PRBCPLASTCA=cenPRBCPLASTCA;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------finished PRBCPLASTCA");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  pbodtcacs=[];  cenPBODTCAC=PBODTCAC;
for PBODTCAC=[cenPBODTCAC*(1.0-delta) cenPBODTCAC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
pbodtcacs=[pbodtcacs PBODTCAC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
```

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    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PBODTCAC=cenPBODTCAC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-----------------------------------------finished PBODTCAC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  plivtcacs=[];  cenPLIVTCAC=PLIVTCAC;
for PLIVTCAC=[cenPLIVTCAC*(1.0-delta) cenPLIVTCAC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
plivtcacs=[plivtcacs PLIVTCAC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PLIVTCAC=cenPLIVTCAC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-----------------------------------------finished PLIVTCAC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  pbodtcohs=[];  cenPBODTCOH=PBODTCOH;
for PBODTCOH=[cenPBODTCOH*(1.0-delta) cenPBODTCOH*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
pbodtcohs=[pbodtcohs PBODTCOH];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PBODTCOH=cenPBODTCOH;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-----------------------------------------finished PBODTCOH");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  plivtcohs=[];  cenPLIVTCOH=PLIVTCOH;
for PLIVTCOH=[cenPLIVTCOH*(1.0-delta) cenPLIVTCOH*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
plivtcohs=[plivtcohs PLIVTCOH];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
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    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PLIVTCOH=cenPLIVTCOH;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-----------------------------------------finished PLIVTCOH");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  pbodtcogs=[];  cenPBODTCOG=PBODTCOG;
for PBODTCOG=[cenPBODTCOG*(1.0-delta) cenPBODTCOG*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
pbodtcogs=[pbodtcogs PBODTCOG];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PBODTCOG=cenPBODTCOG;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-----------------------------------------finished PBODTCOG");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  plivtcogs=[];  cenPLIVTCOG=PLIVTCOG;
for PLIVTCOG=[cenPLIVTCOG*(1.0-delta) cenPLIVTCOG*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
plivtcogs=[plivtcogs PLIVTCOG];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PLIVTCOG=cenPLIVTCOG;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-----------------------------------------finished PLIVTCOG");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  peffdcvgs=[];  cenPEFFDCVG=PEFFDCVG;
for PEFFDCVG=[cenPEFFDCVG*(1.0-delta) cenPEFFDCVG*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
peffdcvgs=[peffdcvgs PEFFDCVG];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
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    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    PEFFDCVG=cenPEFFDCVG;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-------------------------------------------finished PEFFDCVG");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  bmaxkdcs=[];  cenBMAXKDC=BMAXKDC;
for BMAXKDC=[cenBMAXKDC*(1.0-delta) cenBMAXKDC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
bmaxkdcs=[bmaxkdcs BMAXKDC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    BMAXKDC=cenBMAXKDC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------------finished BMAXKDC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kdissocs=[];  cenKDISSOC=KDISSOC;
for KDISSOC=[cenKDISSOC*(1.0-delta) cenKDISSOC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kdissocs=[kdissocs KDISSOC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KDISSOC=cenKDISSOC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------------finished KDISSOC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vmaxcs=[];  cenVMAXC=VMAXC;
for VMAXC=[cenVMAXC*(1.0-delta) cenVMAXC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
vmaxcs=[vmaxcs VMAXC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
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    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VMAXC=cenVMAXC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------------finished VMAXC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  fractcacs=[];  cenFRACTCAC=FRACTCAC;
for FRACTCAC=[cenFRACTCAC*(1.0-delta) cenFRACTCAC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
fractcacs=[fractcacs FRACTCAC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    FRACTCAC=cenFRACTCAC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("------------------------------------------finished FRACTCAC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  fracothercs=[];  cenFRACOTHERC=FRACOTHERC;
for FRACOTHERC=[cenFRACOTHERC*(1.0-delta) cenFRACOTHERC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  fracothercs=[fracothercs FRACOTHERC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    FRACOTHERC=cenFRACOTHERC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("----------------------------------------finished FRACOTHERC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  cldcvgs=[];  cenCLDCVG=CLDCVG;
for CLDCVG=[cenCLDCVG*(1.0-delta) cenCLDCVG*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
cldcvgs=[cldcvgs CLDCVG];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
```

```
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    CLDCVG=cenCLDCVG;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-------------------------------------------finished CLDCVG");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  clkiddcvgs=[];  cenCLKIDDCVG=CLKIDDCVG;
for CLKIDDCVG=[cenCLKIDDCVG*(1.0-delta) cenCLKIDDCVG*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  clkiddcvgs=[clkiddcvgs CLKIDDCVG];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    CLKIDDCVG=cenCLKIDDCVG;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("----------------------------------------finished CLKIDDCVG");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  vmaxlunglivs=[];  cenVMAXLUNGLIV=VMAXLUNGLIV;
for VMAXLUNGLIV=[cenVMAXLUNGLIV*(1.0-delta) cenVMAXLUNGLIV*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  vmaxlunglivs=[vmaxlunglivs VMAXLUNGLIV];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    VMAXLUNGLIV=cenVMAXLUNGLIV;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------finished VMAXLUNGLIV");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kmclaras=[];  cenKMCLARA=KMCLARA;
for KMCLARA=[cenKMCLARA*(1.0-delta) cenKMCLARA*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kmclaras=[kmclaras KMCLARA];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
```

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    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KMCLARA=cenKMCLARA;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-----------------------------------------finished KMCLARA");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  fraclungsyscs=[];
cenFRACLUNGSYSC=FRACLUNGSYSC;
for FRACLUNGSYSC=[cenFRACLUNGSYSC*(1.0-delta) cenFRACLUNGSYSC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  fraclungsyscs=[fraclungsyscs FRACLUNGSYSC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    FRACLUNGSYSC=cenFRACLUNGSYSC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("------------------------------------finished FRACLUNGSYSC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kmtcohs=[];  cenKMTCOH=KMTCOH;
for KMTCOH=[cenKMTCOH*(1.0-delta) cenKMTCOH*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kmtcohs=[kmtcohs KMTCOH];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KMTCOH=cenKMTCOH;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("------------------------------------------finished KMTCOH");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kmglucs=[];  cenKMGLUC=KMGLUC;
for KMGLUC=[cenKMGLUC*(1.0-delta) cenKMGLUC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kmglucs=[kmglucs KMGLUC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KMGLUC=cenKMGLUC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
```

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    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("------------------------------------------finished KMGLUC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kmettcohcs=[];  cenKMETTCOHC=KMETTCOHC;
for KMETTCOHC=[cenKMETTCOHC*(1.0-delta) cenKMETTCOHC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  kmettcohcs=[kmettcohcs KMETTCOHC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KMETTCOHC=cenKMETTCOHC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("----------------------------------------finished KMETTCOHC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kurntcacs=[];  cenKURNTCAC=KURNTCAC;
for KURNTCAC=[cenKURNTCAC*(1.0-delta) cenKURNTCAC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kurntcacs=[kurntcacs KURNTCAC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KURNTCAC=cenKURNTCAC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-----------------------------------------finished KURNTCAC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kmettcacs=[];  cenKMETTCAC=KMETTCAC;
for KMETTCAC=[cenKMETTCAC*(1.0-delta) cenKMETTCAC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kmettcacs=[kmettcacs KMETTCAC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KMETTCAC=cenKMETTCAC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("-----------------------------------------finished KMETTCAC");
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auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kbilecs=[];  cenKBILEC=KBILEC;
for KBILEC=[cenKBILEC*(1.0-delta) cenKBILEC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kbilecs=[kbilecs KBILEC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KBILEC=cenKBILEC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------------finished KBILEC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kehrcs=[];  cenKEHRC=KEHRC;
for KEHRC=[cenKEHRC*(1.0-delta) cenKEHRC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
kehrcs=[kehrcs KEHRC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KEHRC=cenKEHRC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("---------------------------------------------finished KEHRC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kurntcogcs=[];  cenKURNTCOGC=KURNTCOGC;
for KURNTCOGC=[cenKURNTCOGC*(1.0-delta) cenKURNTCOGC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  kurntcogcs=[kurntcogcs KURNTCOGC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KURNTCOGC=cenKURNTCOGC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("----------------------------------------finished KURNTCOGC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  knatcs=[];  cenKNATC=KNATC;
for KNATC=[cenKNATC*(1.0-delta) cenKNATC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];
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auclivtcadms=[auclivtcadms AUCLIVTCADM];  aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];
knatcs=[knatcs KNATC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KNATC=cenKNATC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------------finished KNATC");
auccblddms=[];  auclivtcadms=[];  aucctcohdms=[];  kkidbioactcs=[];  cenKKIDBIOACTC=KKIDBIOACTC;
for KKIDBIOACTC=[cenKKIDBIOACTC*(1.0-delta) cenKKIDBIOACTC*(1.0+delta)];  start @NoCallback;
auccblddms=[auccblddms AUCCBLDDM];  auclivtcadms=[auclivtcadms AUCLIVTCADM];
aucctcohdms=[aucctcohdms AUCCTCOHDM];
sasum_hours=[sasum_hours HOURS];  kkidbioactcs=[kkidbioactcs KKIDBIOACTC];  end;
    sa_auccblddm=((auccblddms(:,2)-auccblddms(:,1))/(delta*2.0)./auccblddms(:,1))*(1.0-delta);
    sa_auclivtcadm=((auclivtcadms(:,2)-auclivtcadms(:,1))/(delta*2.0)./auclivtcadms(:,1))*(1.0-
delta);
    sa_aucctcohdm=((aucctcohdms(:,2)-aucctcohdms(:,1))/(delta*2.0)./aucctcohdms(:,1))*(1.0-
delta);
    sa_auccblddm2=20.0*((auccblddms(:,2)-auccblddms(:,1))./(auccblddms(:,2)+auccblddms(:,1)));
    sa_auclivtcadm2=20.0*((auclivtcadms(:,2)-
auclivtcadms(:,1))./(auclivtcadms(:,2)+auclivtcadms(:,1)));
    sa_aucctcohdm2=20.0*((aucctcohdms(:,2)-
aucctcohdms(:,1))./(aucctcohdms(:,2)+aucctcohdms(:,1)));
    sasum_auccblddm2=[sasum_auccblddm2 sa_auccblddm2];  sasum_auclivtcadm2=[sasum_auclivtcadm2
sa_auclivtcadm2];
    sasum_aucctcohdm2=[sasum_aucctcohdm2 sa_aucctcohdm2];
    KKIDBIOACTC=cenKKIDBIOACTC;  sasum_auccblddm=[sasum_auccblddm sa_auccblddm];
    sasum_auclivtcadm=[sasum_auclivtcadm sa_auclivtcadm];  sasum_aucctcohdm=[sasum_aucctcohdm
sa_aucctcohdm];
    disp("--------------------------------------finished KKIDBIOACTC");
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LIST OF ACRONYMS

AFCEC	Air Force Civil Engineering Center
DCA	dichloroacetic acid
DoD	Department of Defense
DTIC	Defense Technical Information Center
EPA	Environmental Protection Agency
HJF	Henry M. Jackson Foundation for the Advancement of Military Medicine
IRIS	Integrated Risk Information System
MCMC	Markov Chain Monte Carlo
OASD EI&E	Office of the Assistant Secretary of Defense (Energy, Installations and Environment)
PBPK	physiologically-based pharmacokinetic
RfC	reference concentration
SC	sensitivity coefficients
TCE	Trichloroethylene
TSTC	TriService Toxicology Consortium